Simulation of a Small Scale Biowaste Gasification System for Energy Production

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Dissertation submitted in partial fulfillment of a
Philosophiae Doctor degree in Chemical Engineering

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Abstract

Several waste incinerators in Iceland were closed down in 2011/2012 due to environmental problems and health concerns. To date no cost effective and environmentally acceptable replacement has been found for disposing of the waste that was combusted at these facilities up to 2012. As a result, large amounts of waste have been transported by ferry and road to be landfilled or incinerated hundreds of kilometers away (for example routes include from Vestmannaeyjar to Reykjavik or even in some cases Blönduós, with similar long journeys in other remote locations, for example Vestfirðir). The aim of this PhD project was to take steps towards adapting a greener solution developed elsewhere for waste disposal to Iceland. The process is called gasification which is a waste-to-energy technology. The challenges for waste gasification are its adaption to the Icelandic scale, using waste as feedstock and determining operational parameters. Downscaling must be done while still eliminating the pollution problems of incinerators and the cost constraints of small-scale plants.

To overcome these challenges, the experimental and pilot work at the University in Iceland was conducted by modeling and simulation. Described in this thesis is the following modelling and simulation work: An integrated small-scale gasification system with power production unit was simulated by using ASPEN Plus. This model helps to understand under what conditions and in which ways the system can operate. The system's model was used to analyze and assess the potential of adapting gasification-based waste to power systems for conditions in Iceland. The analysis and assessment includes techno-economic and environmental perspectives.

The project's contribution to the field of gasification is the knowledge regarding simulation of small-scale gasifiers as well as the assessment of their performance and various operating parameters. This knowledge is valuable for developing gasification solutions for smaller communities that have similar waste streams and waste disposal challenges.

The results indicate that electricity production from waste gasification could be technically feasible, environmentally, and economic acceptable option replacing incinerators and landfilling sites for waste disposal in Iceland. Among all the studied feedstock alternatives, timber and wood waste are the most beneficial when certain factors are considered. The production of 1 kWh electricity from timber gasification comes with the relatively low global warming potential of 0.07 kgCO2eq, acidification potential of 0.09 kgSO2eq, and eutrophication potential of 0.36 kgNO3eq. The results of techno-economic assessment show that the net present value is positive for a gasification system with the capability to generate greater than 45 kW. Discounted payback period (DPP) will be also lower than 2 years for a gasification with capacity higher than 75 kW. However, it could be lower than 6 months if gasification is applied in capacity greater than 200 kW.

It is also worth to mention that, if cogeneration of heat and power (CHP) is used – instead of only power production – the DPP can be shortened even further (i.e., in cold locations where cheap geothermal hot water is not available) and that will make gasification even more feasible than shown in this thesis.

Útdráttur

Fjölmörgum sorpbrennslum á Íslandi var lokað 2011/2012 vegna dioxin/furan mengunar sem greindist í jarðvegi ásamt kjöt- og mjólkurafurðum. Í dag hefur engin hagkvæm og umhverfisvæn lausn komið í stað sorpbrennslanna. Vegna þessa er óhemju mikið af rusli flutt á hverju ári með ruslabílum langar leiðir eftir þjóðvegum landsins (til dæmis frá Vestmannaeyjum til Reykjavíkur eða jafnvel til Blönduóss) til urðunar eða brennslu. Markmið þessa doktorsverkefnis var að taka fyrstu skrefin í að aðlaga græna sjálfbæra lausn fyrir förgun lífræns úrgangs á Íslandi. Lausnin sem rannsökuð var í verkefninu nefnist gösun. Gösunarkerfi eru sjálfbær úrgangs-til-orku kerfi sem auk þess að umbreyta úrgangi í lífeldsneyti þá lágmarka þau losun mengandi efna. Helstu áskoranir við gösun lífræns úrgangs á Íslandi eru magn- og stærðartakmarkanir, samsetning lífræna úrgangsins og rekstrarstillingar búnaðarins. Við útfærslu á litlum gösunareiningum þarf að huga að bæði rekstrarhagkvæmni og að viðhalda kostum gösunartækninnar framyfir brennslu og urðun t.a.m., minni loft- og grunnvatnsmengun

Til að takast á við þessar áskoranir var útbúið ASPEN Plus líkan af litlu gösunarkerfi með samþættu raforkuvinnslukerfi og það hermt. Líkanið hjálpar til við að skilja við hvaða aðstæður og hvernig reka má kerfið. Kerfislíkanið var notað til að greina og meta kerfið út frá bæði tækni-hagfræðilegu og umhverfislegu sjónarhornum til að geta lagt fram ráðleggingar um hvernig aðlaga má sjálfbært úrgangs-til-orku kerfi að aðstæðum á Íslandi.

Framlag þessa doktorsverkefnis til fræðasviðsins er aukin þekking á hermun smærri gösunarkerfa – ásamt mati á frammistöðu kerfanna og rekstrarbreyta þeirra – í samfélögum sem hafa svipaðar áskoranir í úrgangsmálum. Niðurstöðurnar benda til þess að raforkuframleiðsla með gösun lífræns úrgangs gæti verið fýsilegur, umhverfislegur og efnahagslega ásættanlegur valkostur í stað brennslu og urðunar lífræns úrgangs á Íslandi. Af þeim úrgangi sem var rannsakaður kom timbur og timburúrgangur best út þegar litið til ákveðinna þátta. Framleiðsla á 1 kWst með gasgervingu timburs hefur hnatthlýnunarmátt uppá 0,07 kg koltvísýringsígildi, súrnunarmátt uppá 0,09 kg brennisteinsdíoxíðígildi og ofauðgismátt uppá 0,36 kg nítratígildi. Niðurstöður tækni-hagfræðilegs mats sýna að hreint núvirði er jákvætt fyrir gösunarkerfi sem hefur getu til að framleiða yfir 45 kW. Núvirtur endurgreiðslutími gösunarkerfa með afkastagetu yfir 75 kW verður undir 2 árum og fyrir kerfi með afkastagetu yfir 200 kW verður tíminn undir 6 mánuðum.

Þess er einnig vert að geta að með samþættri varma- og raforkuvinnslu (CHP) – í stað einungis raforkuvinnslu – þá er hægt að stytta núvirta endurgreiðslutímann enn frekar (þ.e. á köldum svæðum þar sem ekki er aðgangur að ódýru hitaveituvatni) og þar með verður gösun enn álitlegri kostur en sýnt er í þessari ritgerð.

Dedication

To my dear mother for her endless love and encouragement

To Movaffaq, my dearest husband, who was always with me with light of hope and support

To Amirhossein, Taha and Yasin, our cute boys that I never force myself to stop loving them

Preface

This thesis is submitted in candidacy for a Ph.D. degree from the University of Iceland. The work has been conducted between Dec 2017 and April 2021 at Faculty of Industrial Engineering, Mechanical Engineering and Computer Sciences supervised by Prof. Runar Unnthorsson and Prof. Christiaan Richter.

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Sahar Safarianbana

April 2021.

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II. Safarian, S., Unnþórsson, R., & Richter, C. (2019). A review of biomass gasification modelling. ***Renewable and Sustainable Energy Reviews***, *110*, 378-391.

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Abbreviations

AP	Acidification potential
C_c	Total capital costs of investment
CF_n	Annual cash flow
C_g	Hardware price
CGE	Cold gas efficiency
CHP	Cogeneration heat and power
$C_{O\&M}$	Operation and Maintenance Costs
DPP	Discounted payback period
E	Expenditures
EP	Eutrophication potential
ER	Equivalence ratio
Eq	Equilibrium
FC	Fixed carbon
GHG	Greenhouse gas
G_p	Syngas yield
GWP	Global warming potential
HHV	Higher heating value
K€	Kilo-euro
Ki	Kinetic
LHV	Lower heating value
M	Moisture
MSW	Municipal solid waste
NPV	Net present value
R	Reaction
RE	Reactor
Sep	Separator
T	Temperature
VM	Volatile matter
W	Power
WTB	Icelandic municipalities pay a fee
r	Discount rate
t	Lifetime of the investment
y	Mole fraction of gas pieces in the syngas
wt%	Weight percent
γ	Yield coefficient
η	Efficiency

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1 Introduction

1.1 Motivation

Waste is a major problem that causes not only serious economic losses, but also significant environmental impacts. Better living standards, tourism activity and economic growth accelerate the waste generation in Iceland. Improper management of waste has led to increased public concerns about health and environmental impacts.

The total amount of municipal solid waste (MSW) in Iceland in 2010 has been estimated to 76 ± 6 thousand ton, based on data available from Sorpa, the waste management company in the Capital area. In other words, the annual amount of MSW per capita has been estimated to 222-257 kg [1]. The amount of MSW produced in 2030 is also estimated to approximately 100 ± 7 thousand ton. Generally, 60% of this amount is organic material which 43, 41 and 16% of that are paper mixed, timber and wood and garden wastes, respectively [1, 2].

Landfilling and incineration have been the only methods of disposal of solid wastes in Iceland, while most landfill sites have been open dumping areas, which pose serious environmental and social threats. In addition, an incinerator in Skutulsfjörður caused carcinogenic and toxic chemicals to be found in meat and milk [3]. Soil and incinerator-emissions measurements at several sites, including Kirkjubaejarklaustur, had recorded emissions 85 times above the EU limit [4]. These problems resulted in the shut-down of several incinerators and the withdrawal of Icelandic meat and milk products [3, 5].

It is worth mention that disposal of solid waste by using landfilling and incinerators is not conducted only in Iceland. In fact, it is an increasing problem in both developed and developing countries. Incineration is among the worst approaches that cities can take to achieve waste reduction goal. It is expensive, inefficient, creates environmental risks and has harmful impacts on human health [6]. Several studies of incinerators have found evidence of an adverse health effect like Kim et al [7] found adverse health effects like cancers in the vicinity of solid waste incinerators in Seoul; Gouveia and Ruscitto [8] investigated various cancers in Brazil; Vilavert et al [9] monitored the concentrations of polychlorinated dibenzo-p-dioxins and dibenzofurans in a region in Spain containing an incinerator; Elliott et al [10] studied cancer of the larynx and lung in Britain; Vinceti et al [11] focused on congenital abnormalities in Italy. All these maters show that this problem exists in numerous locations around the globe, and therefore the solutions are not just for Iceland but carry much broader value even if the case studied here is Iceland.

All these problems demonstrated the need to find more environmentally with less adverse impacts on health alternatives than conventional incineration and landfilling [12, 13]. The

method must be environmentally friendly, low cost, energy efficient and must reduce land use and emissions. These advantages are all found in modern gasification technology. Gasification is an attractive alternative that has recently gained considerable attention, as it disposes of solid waste without landfilling or incineration problems [14-16].

Recovering energy from biomass or organic solid waste requires biochemical and/or thermochemical processes [17]. During biochemical processes like fermentation, biomass is converted to biofuels through the digestive action of living organisms. However, in thermochemical processes, biomass is converted to biofuels, gases, and chemicals by applying heat and/or pressure. Gasification, also widely used to gasify coal and natural gas, is the most prominent thermochemical biomass-to-energy and waste-to-energy conversion processes gaining ever more research and commercial interest [18, 19].

In addition to producing syngas from biomass for subsequent biofuel synthesis, gasification typically achieves superior efficiency for electricity generation compared to more conventional alternatives such as incineration (to generate steam for turbines). Electricity production by utilizing gasification recover more electricity per kilogram of biomass [20] or per kilogram of municipal waste [21-23] compared with alternatives such as incineration or biogas from digesters. Using gas engines, gas turbines or fuel cells, electricity can easily be generated from syngas with existing or marginally modified infrastructure.

In certain situations, the superior energy recovery efficiency of gasification does result in the lowest cost (compared with conventional technologies) in per unit of energy produced from biomass [20, 24]. Hence, the thermochemical or gasification route between raw biomass and energy is significantly more flexible than the currently dominant biochemical route. Gasification can economically transform many more types of biomass compared to fermentation. Demonstrated feedstock include most types of organic waste, sea-weed and forestry waste. The syngas produced from any of these sources is readily processable into liquid fuels or can fire the efficient co-generation of heat and electricity. It is on account of this superior flexibility of gasification, both on the feedstock end and energy generation end, that gasification will likely play an ever-increasing role in our future energy mix.

In gasification, feedstocks such as paper, cardboard, wood is mixed with steam and limited oxygen at high temperature. Unlike the relatively uncontrolled combustion occurring in incineration, in gasification waste is converted to syngas comprising mainly carbon monoxide and hydrogen [25]. Syngas is combustible and can be used as a fuel of internal combustion engines to generate power and hot water or steam (Figure 1.1) [26-29]. In addition, various biofuels can be produced by applying syngas purification and conversion technologies that in this way energy value in the waste and contribution to a sustainable energy supply is increased. For instance, biomethane could be purified after passing of syngas from the methane recovery/capturing plant. Similarly, in another alternative, hydrogen could be purified after passing of syngas from the H_2 recovery/capturing unit. Moreover, biowastes can be converted into bioethanol by passing of syngas from syngas

fermentation and product recovery units. Biodiesel can be also produced through the integrated gasification and the Fischer-Tropsch process.

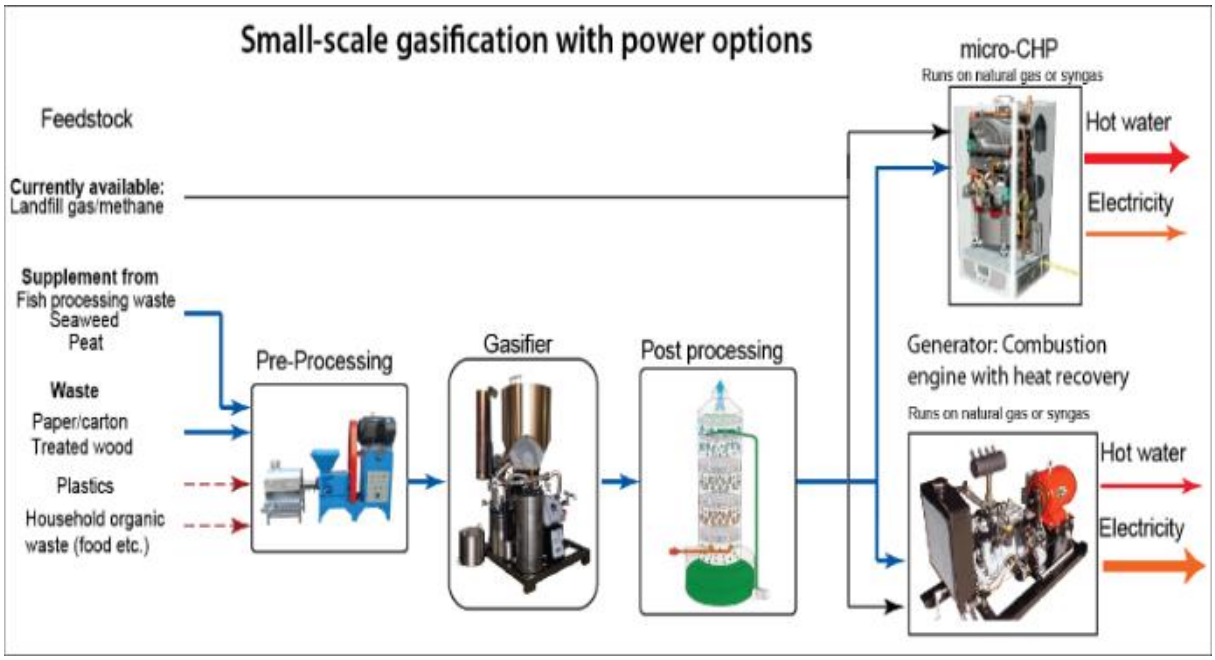


Figure 1-1. The gasification-process configuration

Various researches mention that gasification is an emerging but promising technology, especially in comparison with commercially available technologies like incineration [30-33]. Gasification plants also produce much lower levels of air pollutants [34, 35]. The process also reduces the environmental impact of waste disposal because it utilizes waste as a feedstock and uses less water in comparison with traditional coal-based power plants [34]. Additionally, the by-products of gasification are non-hazardous and readily marketable. Equally important, waste gasification can be implemented as a more reliable energy supply technology for cities or towns that are far from the central energy networks and need to have a district heat and power system [36].

The challenge for local waste gasification is its adaption to the Icelandic scale, feedstock and operational parameters. Downscaling must be done while still eliminating the pollution problems of incinerators and the cost constraints of small-scale plants. The key to develop this technology is to overcome the problems associated with technical and economic aspects of power production especially for small-scale plants as well as environmental acceptance.

Gasification's potential has been proved in medium-scale facilities turning waste into power, such as Averøy in Norway [37]. Only a few successful small-scale studies exist in the literature, but their results increase the probability of applying waste gasification in Iceland. The admissible range of feedstock properties is narrow for each gasifier design, because the chemistry and fluid dynamics of gasification are very sensitive to variations in feedstock composition, moisture, ash content and char [38]. Variation in properties has a major impact on the performance, cost and feasibility of a system [39]. Moreover, various operational

parameters, such as temperature, equivalence ratio, steam injection, air-flow rate and moisture content, have different effects on syngas composition and system efficiency.

The global academic value of this project is that it has provided the detailed knowledge about the simulation modeling of the small-scale gasification, its performance under various conditions and its environmental and techno-economic assessment, to the world where there is after all many other smaller communities with similar waste streams and waste disposal challenges. In addition, as the practical value this project provides encouragement and the required information for implementation of biowaste gasification to the world especially to Iceland that can be used by SORPA or other waste-disposal companies outside Reykjavik, including smaller places such as Vestmannaeyjar and Vestfirðir. It provides a green solution for disposing of significant amounts of waste and for mixing diverse feedstocks, including painted and treated wood (about 40.000 tons per year), without the methane emissions and groundwater leaching of landfilling or the air pollution and toxic residues of incineration. It could lead to a sustainable waste-management system that preserves a relatively pristine environment in Iceland. Moreover, before this project no research has been done on environmental and techno-economic assessment of small-scale waste biomass gasification as well as its integration with power production unit. Beneficially, this project has a practical value that prove the production of electricity from waste biomass gasification linked with power unit could be a feasible, environmentally and economic acceptable option to be implemented instead of incinerators and landfilling sites for waste disposal in Iceland. It can be applied for energy supply in low populated regions in the world that are far from the central energy networks and need to have a district heat and power system.

1.2 Research questions

The aim of this research project was to investigate whether small-scale gasification technology could be made feasible, environmentally friendly and techno-economically viable option for waste treatment and energy production in Iceland. In this manner the author addressed the following set of research questions, which interweaved the conducted study:

RQ1: What were the waste feedstocks that could be fed to the gasifier?

> Here, it was required to find what kind of organic wastes are produced in Iceland that could be feasibly disposed by gasification?

RQ2: What was the best modelling approach?

> In order to accurately predict waste-gasifier performance as a function of feedstock composition, pre-treatment and gasifier settings, it was required to find the most effective method for modeling of the considered system.

RQ3: What were the optimal settings of operating parameters on the gasification technology?

Various operating conditions such as temperature, equivalence ratio, moisture content and waste composition influence on the produced gas composition, overall system efficiency and system performance. Hence, to have a system with optimal performance it was required to evaluate, effects of these operating parameters on the system output trough several sensitivity analyses.

RQ4: What were the effects of several inputs on the power output from the system?

In this part, the effects of various feedstocks and operating conditions on electrical efficiency and net output power from the gasification system integrated with power production unit were evaluated to find the optimal conditions to have a maximum electricity generation.

RQ5: Was the applied system environmentally satisfactory?

In order to find the considered system is satisfied from environmental viewpoint, it was required to carry out an environmental assessment of the system as well as to find at what condition had the minimum environmental impact.

RQ6: Could small-scale gasification be made techno-economically feasible?

Here, it was required to find at what conditions (like system capacities and prices) implementation of gasifier could be economic with positive net present value.

1.3 Contributions

In this project, the potential of the gasification technology for energy production and municipal solid waste (MSW) treatment for small communities in Iceland is explored. The main contributions of this thesis are divided into five major categories that are responses to the above mentioned RQs.

First, diverse types of MSWs are studied and then feedstocks in Iceland that can be feasibly disposed by gasification are identified (response to RQ1). Results of this part were brought as one part of paper I, published in *Energies journal* [5] and are covered in Section 3.2.2 Case study.

Second, all approaches for biowaste gasification modelling are studied to determine which are appropriate based on the type of gasifier, feedstock, operational parameters and tar formation. A detailed methodology characterization that includes consequential modelling choices is introduced and stoichiometric and nonstoichiometric models lead to identical predictions or not are addressed. Moreover, tar modelling in gasification models is studied

and classified in different ways in a given application. The results of this part (response to RQ2) were published in papers II and III in the *Renewable and Sustainable Energy Reviews journal* [40, 41]. Everything about this part have been brought in Section 2.2 Biomass gasification models.

Third, a primary simulation model for biowaste gasification is developed to predict its performance, fluid flow, heat transfer and process patterns and to understand whether, under what conditions and in which ways the system can operate. The results of this part (response to RQ3) were published in papers IV and V at the journal of *Power and Energy Engineering* [42] and also presented and published in the *ASME 2019 International Mechanical Engineering Congress & Exposition* [43]. Results about this part have been brought in Section 4.1 Primary model.

Fourth, an upgraded simulation model is developed for integrated biowaste gasification with power production unit as an attractive method for high efficient electricity generation to assess performance of producing electricity from gasifying of various types of organic wastes in Iceland. The objectives are finding the optimal operating conditions (type of feedstock, gasifier temperature, equivalence ratio and moisture content in biomass) to make highest electrical efficiency. The results of this step (response to RQ4) were brought in published papers VI, VII and X at the *Energy journal* [29] and *International Journal of Applied Power Engineering (IJAPE)* [2, 16]. Results about this part have been brought in Section 4.2 Advanced model.

Fifth, and the final, an environmental assessment and techno-economic analysis of energy recovery through the biowaste gasification are carried out. In this part, a comprehensive assessment of environmental and economic feasibility of the gasification facilities integrated with electricity generation unit are directed to propose a sustainable waste to power system adapted with conditions in Iceland. Moreover, the results of integrated biowaste gasification and power system is compared with waste incineration as a conventional and currently running system in Iceland. Results of environmental assessments (response to RQ5) were published in paper VI at the *Energy journal* [29] and results from techno-economic analysis (response to RQ6) were brought in papers VIII and IX at the journal of *Biophysical Economics and Resource Quality* [44] and *Journal of Power and Energy Engineering* [45]. Results about the environmental assessment have been brought in Section 4.3 Environmental assessment and results about the techno-economic assessment have been talked in Section 4.4 Techno-economic assessment. An overview of the relation between the contributions and the publications can be found in Table 1.1.

Table 1-1. Relation matrix of publication contributions and research questions

Paper / RQ	I	II	III	IV	V	VI	VII	VIII	IX	X
RQ1	X									
RQ2		X	X							
RQ3				X	X					
RQ4						X	X			X
RQ5						X				
RQ6								X	X	

1.4 Outline

The following chapters will provide the thesis structure as follows.

Chapter 1—Introduction presents the motivation and research methodology for answering the research questions posed in this thesis.

Chapter 2—Background provides background on gasification process and technologies as well as a background on biomass gasification modelling approaches.

Chapter 3— Material and methods presents assumptions, applied methods for simulation modeling of the system and description of the case study. This chapter also provides a detail description of the system boundaries, methodology and data required for environmental and techno-economic assessments of the system.

Chapter 4— Results and discussions includes results of the developed simulation models for biowaste gasification integrated with power production unit as well as results of performance analysis of the system based on various inputs and conditions. Moreover, this chapter provides results and discussion about environmental and techno-economic assessments of the system through different sensitivity analyses.

Chapter 5— Conclusions concludes the thesis and presents perspectives for future research opportunities as well as thesis limitations.

Chapter 6— Papers includes the papers published through this PhD project.

2 Background

In this chapter leads with a brief overview and introduction to gasification and the different technology options available. Moreover, various biomass gasification modelling approaches are studied and classified based on the type of gasifier, feedstock, operational parameters and tar formation. Several biomass gasification modelling approaches are reviewed, analysed and a new classification of the most important gasification modelling approaches are proposed. A detailed methodology characterization that includes consequential modelling choices is introduced and stoichiometric and nonstoichiometric models lead to identical predictions or not are addressed. Tar modelling in gasification models is also studied and classified in three ways in a given application.

2.1 Gasification process and technologies

2.1.1 Gasification process

Gasification process consists of the following stages: drying, pyrolysis, oxidation (combustion), reduction (char gasification), and cracking (Figure 2.1) [46].

Typically, the moisture in the biomass feed ranges from 5–60% that during drying step, it is reduced to below 5%. In the pyrolysis step, the biomass is heated from 200 up to 700 °C with limited oxygen or air. Under these conditions the volatile components in the biomass are vaporized. The volatile vapor is a mixture of hydrogen, carbon monoxide, carbon dioxide, methane, tar (heavier hydrocarbon) gases, and water vapor [47]. Tar (a black, viscous, and potentially corrosive liquid at standard temperature and pressure that is predominantly composed of heavy organic and inorganic molecules) and char (a solid residue mainly containing carbon) are also produced during pyrolysis [48]. The oxygen supplied to the gasifier reacts with the combustible substances, producing CO_2 and H_2O. Some of this CO_2 and H_2O subsequently are reduced to CO and H_2 upon contact with the char produced from pyrolysis [49]. Moreover, the hydrogen in the biomass can be oxidized, generating water. The reduction reactions occurring inside the gasifier are endothermic, and the energy required for these reactions is provided by the combustion of char and volatiles. Reduction of the biomass yields combustible gases such as hydrogen, carbon monoxide, and methane through a series of reactions; the main reactions in this category are as follows (Table 2.1) [48, 50]:

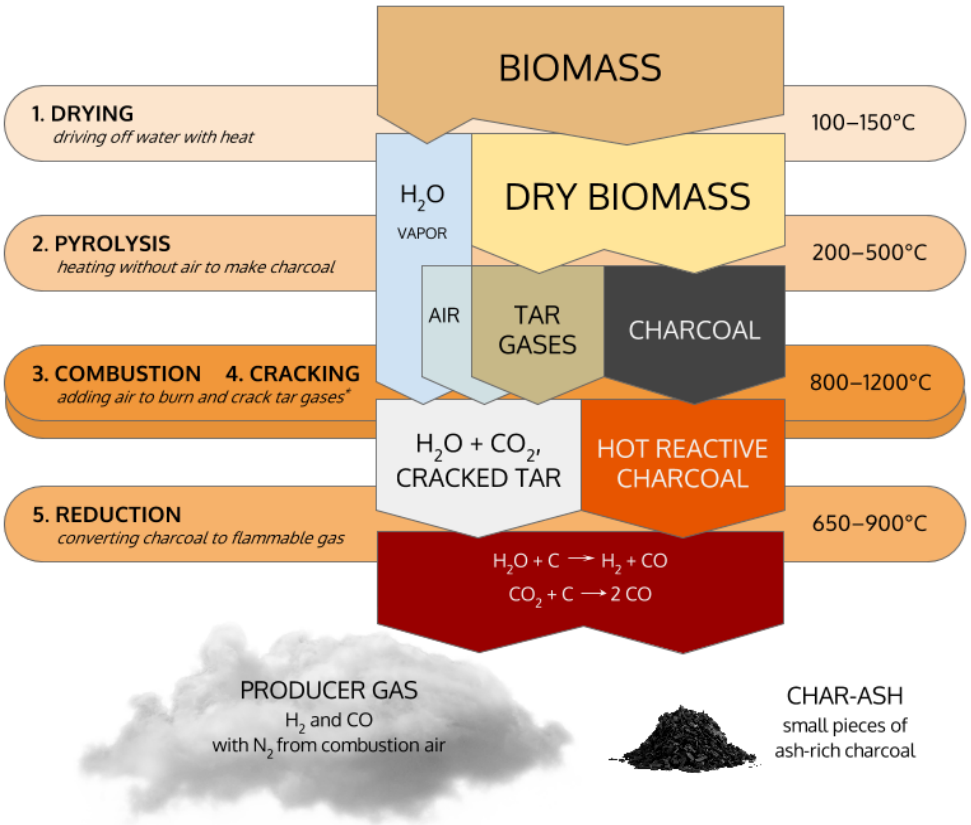


Figure 2-1. Gasification process steps (Reprinted from www.allpowerlabs.com, Copyright 2018 All Power Labs, with permission from All Power Labs)

Table 2-1. Main gasification reactions [48, 50]

Heterogeneous reactions		
$C + O_2 \rightarrow CO_2$ +394 kJ/mol	Complete combustion	R1
$C + 0.5O_2 \rightarrow CO$+111 kJ/mol	Partial combustion	R2
$C + CO_2 \rightarrow 2CO$-172 kJ/mol	Boudouard	R3
$C + H_2O \rightarrow CO + H_2$-131 kJ/mol	Water-gas	R4
$C + 2H_2 \rightarrow CH_4$+75 kJ/mol	Methanation	R5
Homogeneous reactions		
$CO + 0.5O_2 \rightarrow CO_2$+283 kJ/mol	CO partial combustion	R6
$H_2 + 0.5O_2 \rightarrow H_2O$+242 kJ/mol	H_2 combustion	R7
$CO + H_2O \rightarrow CO_2 + H_2$+41 kJ/mol	Water-gas shift (WGS)	R8
$CH_4 + H_2O \rightarrow CO + 3H_2$-206 kJ/mol	Reforming	R9
H_2S and NH_3 formation reactions		
$H_2 + S \rightarrow H_2S$	H_2S formation	R10
$3H_2 + N_2 \rightarrow 2NH_3$	NH_3 formation	R11

Moreover, the tar gases produced during the pyrolysis step undergo cracking in the gasification step, which produces a mixture of non-condensable gasses, light hydrocarbons, and unconverted tar. This process is represented by Equation (1), with γ showing the yield coefficients of the product gasses and unconverted tar. The values of the γ coefficients depend strongly on gasifier operating parameters and feedstock type. However, it is treated as a constant in some works [51]. The most important parameters determining the γ coefficients are temperature, pressure, gasifying medium, catalyst and additives, equivalence ratio (ER), and residence time.

$$tar \rightarrow \gamma_{CO} CO_{(g)} + \gamma_{CO_2} CO_{2(g)} + \gamma_{CH_4} CH_{4(g)} + \gamma_{H_2} H_{2(g)} + \gamma_{tar_{inert}} tar_{inert} \quad (1)$$

An example of a relatively more detailed account of tar cracking, steam and dry reforming, and carbon formation was developed by Devi et al. [52]. Their model utilizes the following reactions:

$$\text{Cracking}: \; pC_nH_x \rightarrow qC_mH_y + rH_2 \quad (2)$$

$$\text{Steam reforming}: \; C_nH_x + nH_2O \rightarrow (n + {}^{x}\!/\!_{2})H_2 + nCO \quad (3)$$

$$\text{Dry reforming}: \; C_nH_x + nCO_2 \rightarrow ({}^{x}\!/\!_{2})H_2 + 2nCO \quad (4)$$

$$\text{Carbon formation}: \; C_nH_x \rightarrow nC + ({}^{x}\!/\!_{2})H_2 \quad (5)$$

Where C_nH_x represents tar and C_mH_y represents dehydrogenated hydrocarbons.

Endothermic reactions decrease the temperature in the reduction zone and the temperature further falls downstream from the gasifier. As a result, most of the tar condenses out in these segments. The resulting tar deposits block and foul engines and turbines, downstream reactors, the syngas conditioning and filtration system. Several efficient methods have been employed to achieve tar removal from the outlet gas. Tar removal technologies can be divided into two approaches: hot gas cleaning after the gasifier (secondary methods) and treatments inside the gasifier (primary methods). Secondary techniques are conventionally used for the treatment of the hot product gas from the gasifier. Tar reduction can be achieved either chemically by using a catalyst or physically by using a cyclone, baffle filter, ceramic filter, fabric filter, rotating particle separator, electrostatic filter, or scrubber. In the primary treatment, the gasifier is optimized to produce a product gas with minimum tar concentration. The different primary treatment approaches are (a) the appropriate selection of operating parameters, (b) use of a bed additive or catalysts, and (c) gasifier modifications. The operating parameters such as temperature, gasifying agent (e.g., air, pure steam, or steam–O_2 mixtures), ER, and residence time play an important role in tar formation and decomposition. By using some active bed additives such as dolomite, olivine, or char inside the gasifier, it is possible to improve the gasifier's performance.

As mentioned, in the pyrolysis step, heat provided by combustion heats the dry biomass to the point that it decomposes into solid char and volatiles (tar and gases). The sum of the tar and gases are equal to the volatile matter (VM), the amount of which is typically quantified using a proximate analysis [51]. The VM percent for different kinds of woody biomasses is high relative to coal, with biomass VM typically in the range of 70–90% by mass. Moreover, char is often modeled as consisting of carbon only, and its amount would be equal to the fixed carbon extracted from the proximate analysis [53]. The typical mass fraction division of the streams within the pyrolysis and gasification steps is depicted in Figure 2.2. The mass flow distribution in this illustrative example are based on the gasification of Olive Wood in a fixed bed downdraft gasifier with air as agent, as reported by Antonopoulos et al [54]. It can be seen that in this particular case, well more than 90% of a downdraft gasification input mass end up in the syngas product stream, while the final tar content in this example is about 0.1% (in general it ranges from 0 to 5%) of the inserted wood material. Hence, the tar amount can be almost negligible in many applications especially if pyrolysis tar is combusted, cracked and reduced.

Pyrolysis of biomass and wood gasification produce about 10 to 30 wt% char and tar in (e.g. [55]). The 10 wt% char and 5 wt% tar produced from olive wood pyrolysis reported by Antonopoulos et al [54], which is shown in Figure 2.2, may be on the low end. The amount of tar that exits either with the product gas, or condenses out on downstream components, depends significantly on the gasifier type and operating conditions and even factors such as the amount of char present in the reduction zone (which can be catalytic for tar cracking and reduction [55-57]). For example, Baker et al. conducted an early survey that found tar yield up to 12 wt% for some updraft gasifiers and in the range of 4–15 wt% for fluidized bed gasifiers, with the higher end observed at lower temperatures (600 °C) [57]. Downdraft gasifiers operating at a relatively higher temperature of 900 °C tend to perform well in terms of final tar yield, with a final tar yield less than 1 wt% common [54, 57].

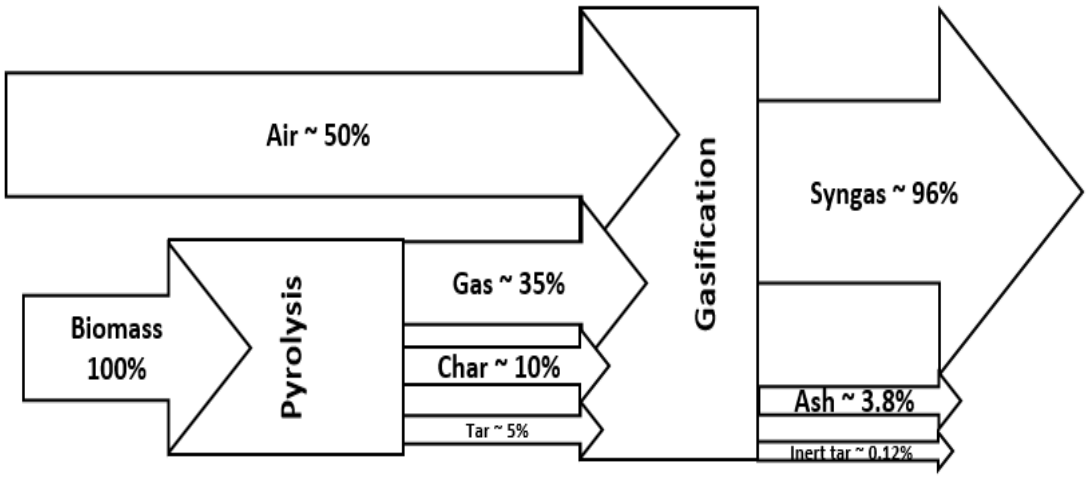


Figure 2-2. A Sankey chart of mass flow distribution throughput biomass gasification

2.1.2 Gasification technologies for biomass

Gasifiers can be divided into two principal types of fixed beds and fluidized beds.

- Fixed-bed (updraft, downdraft, cross-draft): The fixed-bed gasifier category includes gasifiers with a bed filled by solid fuel particles where the gasifying media and gas either are rising (updraft), descending (downdraft), or flowing horizontally through the reactor (cross-draft) [50]. The gasifying media may be air, steam, oxygen, or a mixture of them. The two main practical advantages of fixed-bed gasifiers are that they are relatively more cost-effective for small-scale applications and tend to produce a clean product gas with low dust and low tar content when compared with fluidized bed alternatives [58]. The main disadvantage is that they can have poorer heat transfer and temperature inhomogeneity, and they do not scale up as well as fluidized bed gasifiers. Secondly, fixed-bed gasifiers typically require tighter feed specifications – for example a moisture level below 20% and a fairly uniform particle size distribution with few fines for the biomass (to prevent clogging and channeling) [59, 60].
- The fluidized bed (bubbling, circulating): A typical fluidized bed is a cylindrical column that contains particles and through which fluid—either gaseous or liquid—flows [61, 62]. The velocity of the fluid is sufficiently high enough to suspend the particles within the column, providing a large surface area for the fluid to make contact with, which is the chief advantage of fluidized beds. The main potential advantages of fluidized beds are their superior heat and material transfer between the gas and solid phases [63]. Thus, a fluidized bed maintains a homogeneous temperature field and is more flexible in the sense of wide variations in fuel quality. The main downside of fluidized bed gasifiers is that they tend to produce more dust and particulates in the product gas, which can present a significant problem for downstream equipment [64].

2.2 Biomass gasification models

The performance of the gasification process can be influenced by many factors, including feedstock, process design, and the operating parameters [65]. As a result, gasifier reactors need to be designed either by experimental data and/or by using mathematical or simulation based modelling of the gasification process. The experimental option, though the most reliable, is best utilized in combination with modelling [66]. In practice modelling always play a key role both in applied gasification R&D work or in more fundamental research studies. When it comes to the applied work models that are validated through experiments do reliably predict gasifier performance as a function of feedstock and give qualitative and quantitative information for prospective practical operations. Modelling is very effective in optimizing the operation of an existing gasifier, as well as in exploring operational limits and gaining insight into the relationship between operational parameters and in explaining trends in the data [49]. Simulations also serve as a low-cost method for exploring the

potential benefits, costs, and risks associated with the implementation of gasification given the fact that time and budgets for experimentation and pilot data collection are always finite [66].

The main two categories of gasification models are equilibrium and kinetic models. The survey of gasification modelling choices found that roughly 66% biomass gasification simulations utilize some type of equilibrium model, and the remaining 34% utilize some type of kinetic model (Figure 2.3) [41]. Features and weakness of these methods are gathered in Table 2.2 [50, 66, 67].

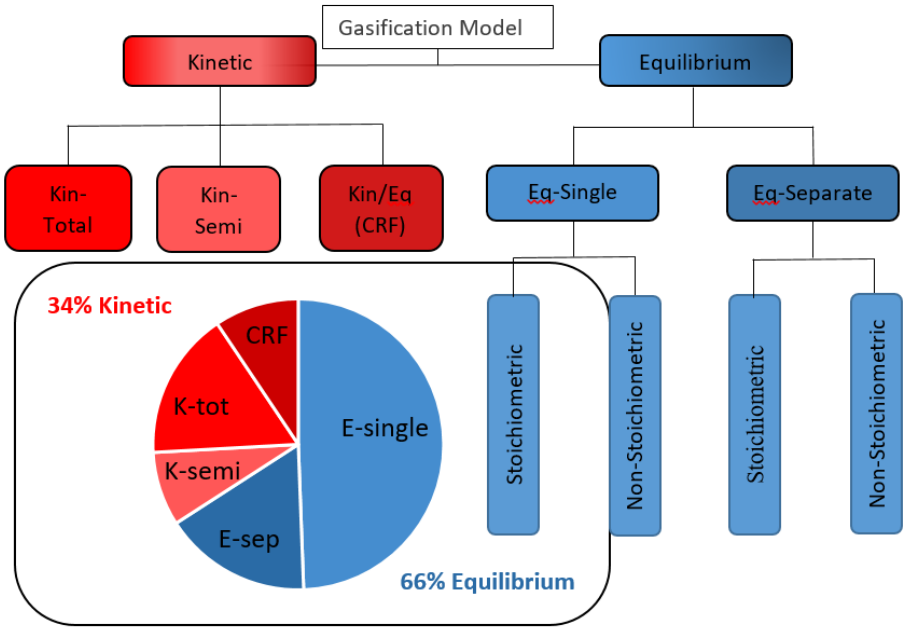


Figure 2-3. A categorization of gasification model types

Table 2-2. Features and weakness of gasification modelling approaches

	Features	**Weakness**
Equilibrium modelling	• Simple method • Not required to consider chemical reactions • Useful tool to evaluate a complex reacting system that is difficult or unsafe to produce experimentally or in commercial operation	• Assumption that the components react in a fully mixed condition for an infinite time period • Assumption that the reactor is zero dimensional • Tars are not considered • Heat loss is neglected

	• Predicts the maximum achievable yield of the products • Very useful in the predicting of downdraft gasifiers • Useful tool for a preliminary comparison of fuels and process parameters • Independent of gasifier design • Flexible for various feedstocks and process parameters • Good representation for high temperatures (750–1000 °C) • Can be improved by using the coefficients for equilibrium constants or yields distribution	• Not fully attained for low operation temperatures • Limitation is for fluidized bed gasifiers • Cannot give highly accurate results for all cases
Kinetics modelling	• Consideration of finite time or finite volume • Accurate and detailed results • Good approximation at low temperatures • Includes both reactions kinetics and hydrodynamics inside the gasifier • Very useful tool for the evaluation of particle size impact • Proper for fluidized bed gasifiers • Able to predict the product composition at different positions along a reactor	• Sensitive to the gas–solid contacting process • Computationally intensive • Limits their applicability to different plants

2.2.1 Thermodynamic equilibrium models

The thermodynamic equilibrium approach predicts the composition of the outlet gases based on the assumption that the components react in a fully mixed condition for an infinite period of time [67, 68]. Thermodynamic equilibrium calculations are simple compared with kinetic models and independent of the gasifier design, and in the simplest, most ideal case, general thermodynamic properties can be used for equilibrium modelling, while a larger set of hard-

to-come-by and accurate kinetic parameters is needed for kinetic modelling. These considerations render equilibrium modelling the more convenient method with which to study the general relations between fuel and process parameters and limiting syngas composition and yield. However, thermodynamic equilibrium may not be achieved in certain gasifiers and under many operating conditions, especially for gasifiers with relatively low operating temperatures [20, 50, 68].

2.2.1.1. Stoichiometric vs Non-stoichiometric models

In the stoichiometric case, the equilibrium of a preselected set of reactions are computed, while in the nonstoichiometric case, the equilibrium of a preselected set of chemical species are calculated. In both cases, thermodynamic property data is used to compute the predicted equilibrium composition that will exit the gasifier.

The steps for the stoichiometric method are the following: 1) Select the reactions to be included in the simulation (in principle, the dominant reactions assumed sufficient to provide a useful estimate of the product gas compositions), 2) then calculate the equilibrium constants of these reactions at the reaction temperature, and 3), finally, compute the overall chemical equilibrium composition for a given feed composition (and pressure).

The explicit steps for the nonstoichiometric method are as follows: 1) Select all the species to be included in the simulation (in principle, all the chemical species that the modeler deems might be in the gasifier effluent in non-negligible amounts) and 2) then compute the resulting minimum Gibbs energy distribution among these chemical species for a given feed composition (which can be specified simply as the elemental composition of the feed [68, 69]) at the reaction temperature and pressure.

At this point, a key question is the following: Which of the two methods will better predict the composition of gasifiers that conform to assumptions 1 to 3? Or, alternatively, will the two methods always predict the same identical equilibrium composition? To clarify this situation, and the roughly even split in the literature as to whether these two approaches necessarily lead to identical results or not, a mathematical proof [40] has been published that shows for the gas phase equilibrium the exact solutions to the stoichiometric and nonstoichiometric models are identical. Hence, if a stable and consistent numerical algorithm is used the equilibrium predicted by both methods (S and NS) will be identical.

The choice between the stoichiometric or the nonstoichiometric method in modelling the basic gasification system is therefore purely a matter of expediency. These approaches are two different methods that converge to the exact same predicted composition. (The exception to this may be more complicated systems than those typically encountered in gasification modelling; systems where there is a subset of reactions that do approach equilibrium and a subset of reactions that do not and where this subset of non-equilibrium reactions limits the product yield.)

2.2.1.2 Eq-single vs Eq-separate models

In addition to stoichiometric or nonstoichiometric, equilibrium models can be classified as Eq-sep (e.g. [54, 60-62, 70-75]) or Eq-sing (e.g. [17, 65, 76-90]) approaches. This classification is based on whether as in the Eq-sep case the char combustion is modeled as achieving a separate and distinct equilibrium independent of the reduction of the VM and un-combusted char, or alternatively (in the Eq-sing case) the combustion and reduction reactions achieve a single global equilibrium as one reactive chemical system.

Schematics of the process flow within the algorithms for each type is shown in Figures 2.5 and 2.6. It can be seen that the Eq-sep approach assumes equilibrium only between the volatile components (produced in the pyrolysis step) and the char that is not combusted. Typically, either the fraction of char combusted, or reduction zone temperature is a model input parameter. The Eq-sep approach thus models char combustion as occurring separately in a second heterogeneous reactor with heat flow from the second exothermic combustion reactor into the first gas-phase reactor. With the Eq-sing approach, the combustion and gasification of both the char and volatile gasses are modeled in a single reactor where a single overall heterogeneous equilibrium is assumed between all the components and all the reactions (combustion reactions and reduction reactions).

For both models the first step is modelling pyrolysis. The pyrolysis step is an extremely complex part of the gasification cycle, having a large number of chemical and physical phenomena occurring rapidly and simultaneously. Generally, when dried biomass is heated in across a temperature range of 200–500 ˚C during the pyrolysis step, the biomass decomposes into solid char and volatiles (tar and gases) as shown in Figure 2.4 [51]. For all model types the relative amounts of VM, char (also called fixed carbon) and ash (inert solid carbon) are typically computed based on empirically motivated input parameters. Within a stoichiometric model there needs to be a formula, or model, that determine not just the amount but also the molecular distribution of VM species produced by pyrolysis. The typical choice is to include H_2O, H_2, CO, CO_2, CH_4, N_2. Sometimes minor or trace elements like Cl_2, NH_3, H_2S and SO_2 etc. is also included if modelling the fate of the relevant elements and species are of interest. In both models char is also specified as a fraction of inert carbon produced in pyrolysis.

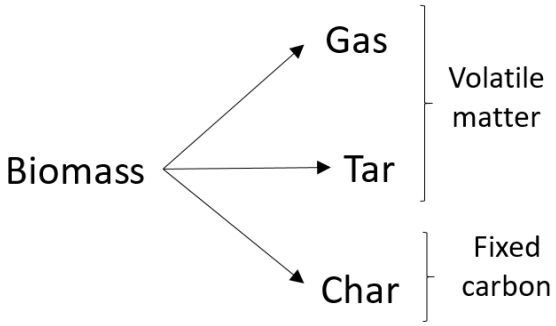


Figure 2-4. Decomposed outputs of biomass through the pyrolysis

The pyrolysis outputs are not separated from each other in Eq-sing simulations. All three types of outputs in Figure 2.4 enter the virtual gasifier (reactor in the model) together. The gasifier is a module that computes the global equilibrium of the gasification reactions based on the stoichiometric or nonstoichiometric approaches. A process flowchart of Eq-sing modelling is shown in Figure 2.5.

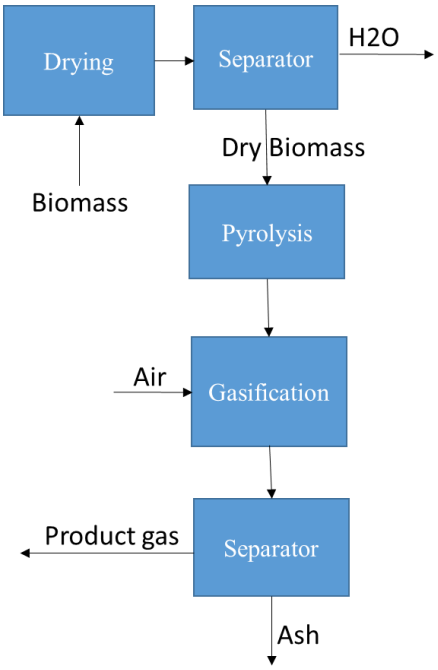


Figure 2-5. Schematics of the process flow within the Eq-sing model

In the Eq-sep model, char is typically subdivided into the fraction of char that will be combusted and the remainder. This fraction can either be specified or internally calculated if the gasifier temperature is specified. Hence the fraction of char to be combusted is separated from the volatile materials and sent to the char combustion reactor with air. Char combustion produces heat that supports most of endothermic gasification reactions, as well as the energy required by the drying and pyrolysis parts (i.e. any of these models include heat transfer from the combustion reactor to the pyrolysis and gasification reactors or computation blocks). The residual solid char (char not fed to the combustion reactor) is fed together the VM and remaining air to the relevant equilibrium reactor modelling gasification step (combustion and reduction zone).

The gasifier equilibrium is computed based on the equilibrium constants (stoichiometric method) or minimization of Gibbs free energy (nonstoichiometric approach), and the combustor is modeled based on combustion equations (Table 2.1). The combustion is typically assumed to be complete. Finally, in most simulations, all unreacted char and ash is separated from gas components of the product stream(s) using a virtual cyclone(s).

As can be seen in Figure 2.6 the Eq-sep model was likely developed to model dual bed gasifiers, where combustion indeed physically happens in a separate chamber than reduction.

But, subsequent researchers also started using the Eq-sep approach for single bed gasifiers where combustion and reduction happens in the same reactor.

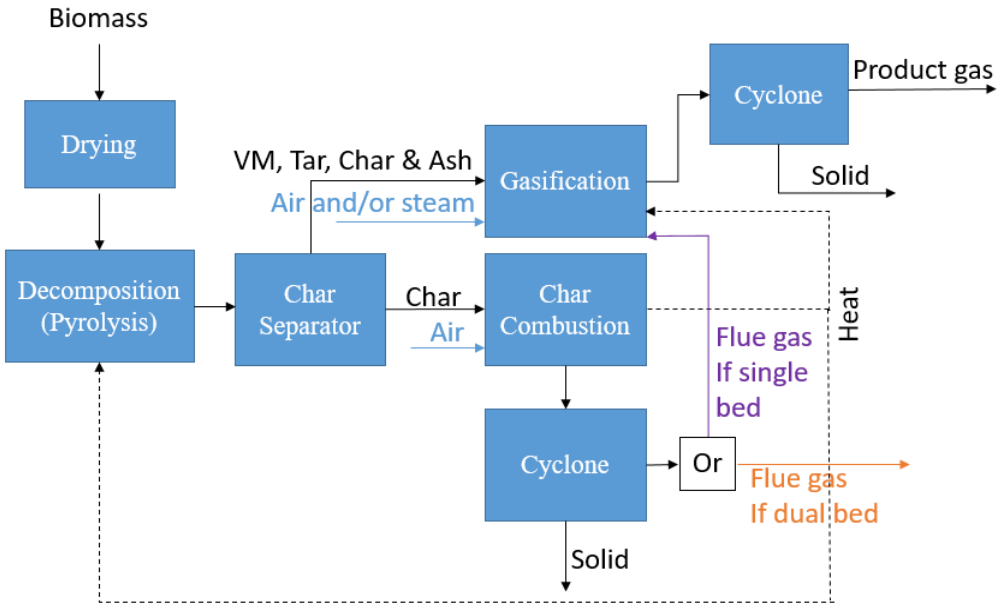


Figure 2-6. Schematics of the process flow within the Eq-sep modelling

The Eq-sing and Eq-sep models each have their own advantages and disadvantages. Eq-sing models are simpler in formulation however they frequently fail to yield satisfactory predictions of experimental gasification outputs. This failure is often attributed to the possibility that complete thermo-chemical equilibrium between all solid carbon (char atoms) and all gas-phase species may not be a realistic assumption for any given real-world gasifier. The notion of incomplete heterogeneous (solid-gas) equilibrium does explanation under prediction of equilibrium simulations of the amount of the residual char (or ash) produced in experiments. That is, for typical gasifiers, all gas-phase reactions and the gas-solid reactions most likely do not approach a single, perfectly global heterogeneous equilibrium where all solid phase atoms are accessible to all reactions. However, equally common deviations between equilibrium simulations (in particular ideal Eq-sing simulations) and experiments are the under prediction of the amount of CH_4 and/or CO_2 produced and an over prediction of the amount of CO and H_2 produced.

2.2.2 Kinetic models

To precisely predict the non-equilibrium product distributions, kinetic modelling is required. Kinetic models can also predict gas composition and temperature profiles throughout the various gasifier zones as well as the evolution of these variables in time during non-steady-state operations and start-up. Because kinetic models have spatial resolution, they by necessity require detailed fluid dynamic modelling in addition to the kinetic model. In general, kinetic modelling can include not only the reaction kinetics and transport but could also include a model of the particle size distribution (and its evolution through the gasifier),

micro-scale mass transport (e.g. diffusion into char particles) and mixing inside the gasifier. Notwithstanding this complexity that is potentially necessary to capture all the consequential physics.

Kinetic models can be very accurate and detailed, but this accuracy is difficult to achieve in practice since these models attempt to describe very complex phenomena, such as gas-solid-particulate fluid flows, gas–solid contacting process and microscopic evolution of particle distributions, which is hard to model reliably. There is however significant ongoing work aimed at developing the detailed kinetic and CFD models and rate laws required to accurately describe the reaction rates and transport of gasification. This work, by individual contributors or groups like for example the CRECK consortium or Reacting Gas Dynamics Laboratory [91, 92], span ab initio methods and experimental approaches [92-105]. However, in the case of fluidized bed gasifiers complex solid–fluid contact patterns result in large deviations from ideal equilibrium compositions (and ideal mixing), and hence for fluidized bed gasifiers the detailed kinetics need to be combined with realistic hydrodynamic modelling; kinetic-hydrodynamic modelling therefore is a particularly common and necessary approach chosen for modelling fluidized bed gasifiers, as argued by several authors [51, 63, 106-112]. As suggested, kinetic models can be divided into Kin-semi (e.g. [51, 107, 108]), Kin-total (e.g. [109, 111-119]), and Ki/Eq (CRF) (e.g. [110, 120-124]) approaches.

The Kin-semi approach assumes local equilibrium for some reactions and gasifier zones but computes kinetically controlled concentrations and temperatures for other zones and reactions. The Kin-semi approach separates char from volatile matter (Figure 2.7(a)) [51, 63, 106, 125, 126]). In this typical type of model, the volatile matter generated in the pyrolysis step first enters a volatile reactions module where a homogenous gas-phase equilibrium is computed by equilibrium constants or the minimization of Gibbs free energy. This equilibrated gas mixture is then fed, together with air/oxygen and/or steam and the solid char, into a kinetic module (which can be CSTR or a PFR) where reaction rate kinetics are used to determine the final composition from the reduction zone and where char gasification occurs[51, 108, 127]).

Within Kin-total models, reaction rate kinetics simultaneously model both the volatile and char gasification reaction rates and local temperature and composition as the simulation code step through the reactor (which can be of any type, with the CSTR or PFR being the most common). Kin-semi models require less kinetic rate laws and parameters than Kin-total models. As a result, Kin-semi models can be more accurate than Kin-total models if the reactor conditions are such that the gas phase is close to the chemical equilibrium. Conversely, Kin-total models with reliable rate laws and hydrodynamic models are, in principle, the only option that could accurately describe non-ideal reactors and operating conditions.

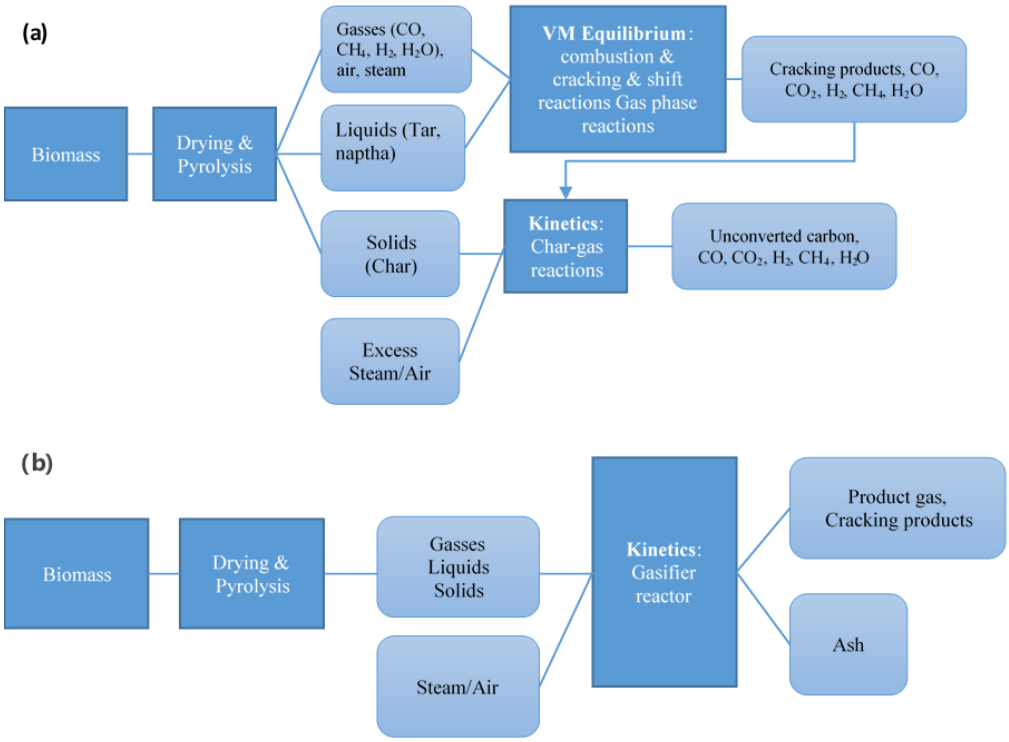


Figure 2-7. Schematics of the process flow within (a) Kin-semi model, (b) Kin-total model

2.2.3 Kinetic/Equilibrium (CRF)

One further modelling approach for biomass gasification is (Ki-CRF) that does not fit neatly into either of the equilibrium categories or kinetic model categories considered this far. Unlike the Kin-semi method, the Ki-CRF approach models the reduction zone kinetically (i.e., all reactions and species concentrations are computed with a PFR-style rate law-based reactor model). However, the rate equations used in the reduction are typically formulated as a relatively simple Arrhenius type reversible reaction that includes the equilibrium constants in the rate expressions to make all the equations thermodynamically consistent. Additionally, the pre-factors of these rate expressions for the reactions involving char are typically empirically adjusted by multiplying them with an adjustable parameter called the char reactivity factor (CRF). As such, this approach is a true hybrid of kinetic reactor modelling, thermodynamic equilibrium data, and empirical adjustments.

Ki-CRF models are designed to model gasifiers where the chemical composition of the product gas is not equal to the equilibrium composition, as is, for example, common with fluidized bed gasifiers. Ki-CRF models furthermore acknowledge the reality that truly reliable rate laws for especially heterogeneous char gasification reactions may not be available and that it may be more expeditious to utilize general thermodynamic equilibrium data and empirical CRFs in relatively simple rate expressions.

Generally, pyrolysis and cracking reactions are not considered in these models because the number of possible pyrolysis products with all the possible reactions and intermediate

products would make the model very complex. Moreover, Ki-CRF models start at the top of the reduction zone, so all the gasification calculations would be based on an empirical estimate of the initial feed into this section. Hence, the accuracy of the model is limited by the availability of data on the initial conditions at the top of the reduction zone.

Finally, terms and conditions of employing different modelling approaches are shown in Table 2.3. As it shown, Equilibrium modelling methods can only be used to predict reliably fixed-bed gasifier performance as a function of feedstock and given information about operational conditions. Kinetic modelling approaches can also present good approximation for fluidized-bed gasifiers at low temperature. Ki-CRF models can be also applied when reliable rate laws for especially heterogeneous char gasification reactions are not available and that it may be more expeditious to utilize general thermodynamic equilibrium data and empirical CRFs in relatively simple rate expressions. Regarding to the above mentioned matters, the method has been used for simulation modeling of the downdraft biomass gasification in this project is equilibrium-based approaches that much more details about it have been explained in the next section.

Table 2-3. Terms and conditions of using different modelling approaches

Modeling approaches	Terms of use
Eq-single	• Using Fixed-bed gasifier • Feedstock with low Tar content • High operating temperature (750–1000 °C) • Lack of information about chemical reactions
Eq-separate	• Using Fixed-bed gasifier • Feedstock with low Tar content • High operating temperature (750–1000 °C) • Existence of information about chemical reactions
Kin-semi	• Using Fluidized-bed gasifier • Low to medium operating temperature • Lack of data about reactions kinetics and hydrodynamics for combustion, cracking, shift reactions and gas reactions
Kin-total	• Using Fluidized-bed gasifier • Low to medium operating temperature • Existence of data about reactions kinetics and hydrodynamics trough all parts of gasifier
Kinetic/Equilibrium (CRF)	• Using Fluidized-bed gasifier • Unavailability of truly reliable rate laws for especially heterogeneous char gasification reactions • Existence of empirical estimate of the initial feed into the gasifier

3 Material and methods

3.1 Primary model

In this part, the developed simulation model for waste biomass gasification to produce syngas is presented and all results of this part have been published in Papers IV and V [42, 43]. The objective from developing the primary model is to evaluate effects of various operating conditions such as temperature, equivalence ratio, moisture content and waste composition on produced gas composition, overall system efficiency and system performance through several sensitivity analyses. Aa a main result of this part, the optimal range of operating conditions for each system with effective performance are gained.

As a primary model, a new equilibrium model based on stoichiometric approach has been developed for the downdraft air gasifier of waste biomasses by using ASPEN Plus version 10. The developed Aspen Plus model involves the following steps: specification of stream class, selection of property method, determination of the system component from databank, specification of the conventional and non-conventional components, specifying the process flowsheet by using unit operation blocks and connecting material and energy streams, defining feed streams (flow rate, composition, and thermodynamic condition) and Specifying unit operation blocks (thermodynamic condition, chemical reactions, etc.).

3.1.1 Assumptions

The following assumptions are employed in the simulations of waste biomass gasification and they were also considered in other researches.

(1) The model is a zero-dimension calculation at steady state, kinetic free and isothermal.

(2) All gases are ideal gases, including hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), steam (H_2O), nitrogen (N_2) and methane (CH_4) [51, 59].

(3) Char contains only carbon and ash in solid phase [51].

(4) Tar and other heavy hydrocarbons are not considered due to the type of gasifier studied in this project [53, 54].

(5) Operation at atmospheric pressure (~ 1 bar) [59, 60, 87].

(6) No heat and pressure losses occur in the gasifier [59, 60, 87].

(7) Simulation is based on stoichiometric approach and by considering the main reactions [73] of R1, R2, R4, R5 and R7 in Table 2.1.

3.1.2 Physical property method

Penge Robinson equation of state with Boston-Mathias alpha function (PR-BM) has been used to estimate all physical properties of the conventional components in the gasification process. This method is suitable for the nonpolar or mildly polar mixtures such as hydrocarbons and light gases and the parameter alpha in this property package is a temperature dependent variable that could be helpful for the correlation of the pure component vapor pressure when temperature is quite high. Moreover, the enthalpy and density model selected for both biomass and ash which are non-conventional components are HCOALGEN and DCOALIGT. MCINCPSD stream containing three substreams comprising MIXED, CIPSD and NCPSD class, was also used to define the structure of simulation streams for the components of biomass and ash which are not available in the standard Aspen Plus component database.

3.1.3 Model description

Figure 3.1 shows the flow chart of waste biomass gasification simulation by using ASPEN Plus based on the stoichiometric approach and Table 3.1 gives the brief descriptions of the unit operations of the blocks used in the simulation. The BIOMSS stream was defined as a nonconventional stream and it was created by inputting of elemental and gross compositions of wastes feedstocks obtained from proximate and elemental analyses. In the next step, RYIELD, the ASPEN Plus yield reactor, was used to simulate the decomposition of the feed. In pyrolysis/decomposition stage, the feedstock was transformed from a non-conventional solid to volatile materials and char. The volatiles included carbon, hydrogen, oxygen and nitrogen and the char was converted into ash and carbon, by specifying the product distribution based on the proximate and ultimate analysis of the waste biomasses. The yield of volatiles was equal to the volatile content in the fuel according to the proximate analysis [63, 80, 128]. For stoichiometric equilibrium simulation of the combustion and gasification parts, REquil reactor was used in which homogeneous and heterogeneous reactions can be defined, simultaneously. However, due to the limitation of ASPEN Plus that each REquil can only contain one heterogeneous reaction, 4 REquil reactors (RE1-RE4) were considered for 4 heterogeneous reactions of R1, R2, R4, R5 (based on Table 1). Two FSplit blocks were used for dividing of volatiles and air streams among reactors of RE1, RE2 and RE3. Then two Mixer blocks were applied to mix outlet gasses and unburned carbons from the up and bottom of reactors, respectively; the product streams called OUTGAS and CARBON, respectively. Then, OUTGAS and CARBON streams with the rest of air stream were entered to RE4 for the heterogeneous reaction of R5 and homogenous reaction of R7. Eventually, the product gas called SYNGAS was exited from the up of RE4.

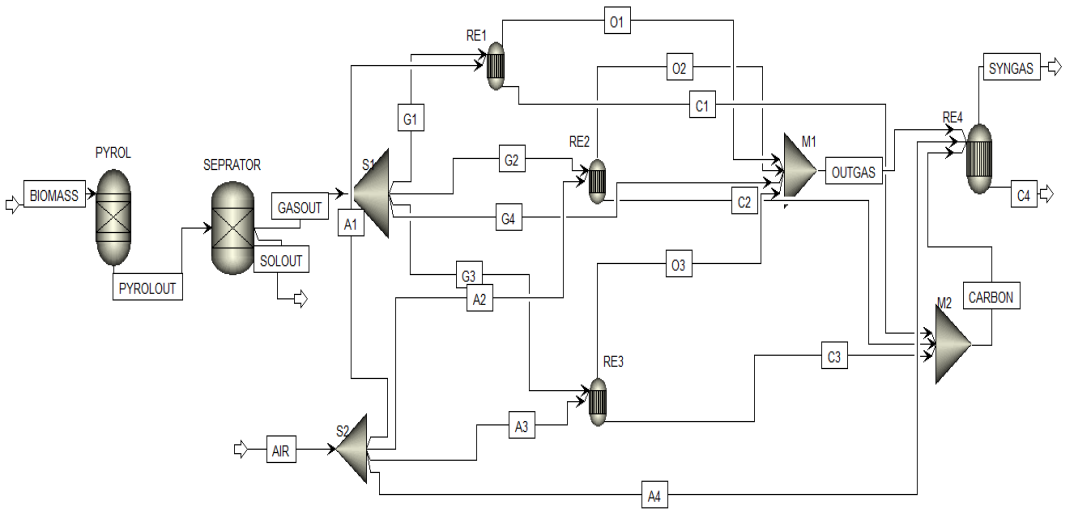


Figure 3-1. Flow chart of the primary simulation model developed by using Aspen Plus for biowaste gasification

Table 3-1. Description of ASPEN Plus unit operation blocks used in model

ASPEN Plus name	**Block name**	**Description**
Ryield	PYROL	Decomposition of non-conventional biomass to conventional components according to its proximate and ultimate analyses.
Requil	RE1, RE2, RE3, RE4	Rigorous equilibrium reactor based on stoichiometric approach.
Sep	SEPRATOR	Gas separation from ash by specifying split fractions.
FSplit	S1, S2	Dividing of gas stream and air stream based on split fractions by S1 and S2, respectively
Mixer	M1, M2	Blending of gasses and carbons into one stream by M1 and M2, respectively

3.2 Advanced model

3.2.1 Model description

In this part, the developed advanced simulation model for waste biomass gasification integrated with power production unit to produce electricity as output of the system is presented and all results of this part have been published in Papers VI, VII and X. The objective from this part is to evaluate the effects of various feedstocks and operating conditions on electrical efficiency and net output power from the gasification system integrated with power production unit to find the optimal conditions to have a maximum electricity generation.

In order to upgrade the primary model, several modifications and complementary technologies were added to the base model. The improved gasification system consists of drying, pyrolysis, combustion and gasification and it is integrated with power production unit as well as heat recovery system. Figure 3.2 shows the flow chart of the advanced waste biomass gasification simulation using ASPEN Plus.

Generally, the moisture in biomass ranges from 5% to 60% that it is reduced to lower than 5% during drying which occurs at a temperature of 150 °C. This step is directed by the stoichiometric reactor RSTOIC in Aspen Plus. This particular module is used to perform chemical reactions of known stoichiometry [128, 129]. The key operation for this step is performed by writing a FORTRAN statement in the calculator block. RSTOIC converts a part of feed to form water which requires the extent of reaction known as [77]:

$$Feed \rightarrow 0.0555084 H_2O \tag{6}$$

In this step, the moisture of each feedstock is partially evaporated and then separated using a separator model, (model id: SEP1). After being stripped from moisture, RYIELD, the yield reactor is used to simulate the decomposition of the feed. In the pyrolysis step, the feedstock is converted to volatile materials (VM) and char. VM includes carbon, hydrogen, oxygen and nitrogen; Char is also converted into ash and carbon, by specifying the product distribution based on the proximate and ultimate analysis of the feedstock [42, 130-132]. Then RGibbs is used to simulate gasification of the biomass. The reactor calculates the syngas composition by minimizing the Gibbs free energy and assumes complete chemical equilibrium. The decomposed feed and air enter the RGibbs reactor where partial oxidation and gasification reactions occur. Another RGibbs reactor is also used in the combustion section with minimum air mixing. Principally, this process is also based on minimization of the Gibbs free energy. The combustion chamber is followed by a gas turbine [133-135]. The thermal content of the gas, obtained as the heat of combustion is removed and used to convert water to high pressure steam though a HEATER. The generated steam finally drives a steam turbine and produces additional power [136]. The solid lines in Figure 3.2 stand for the mass streams, whereas the dashed lines are for the heat streams. The system is assumed to be auto-thermal so that a part of the biomass is combusted inside the gasifier in order to provide the

heat required in situ. Heat is also provided by the hot product gas, as well as the combustion chamber, and is utilized wherever needed.

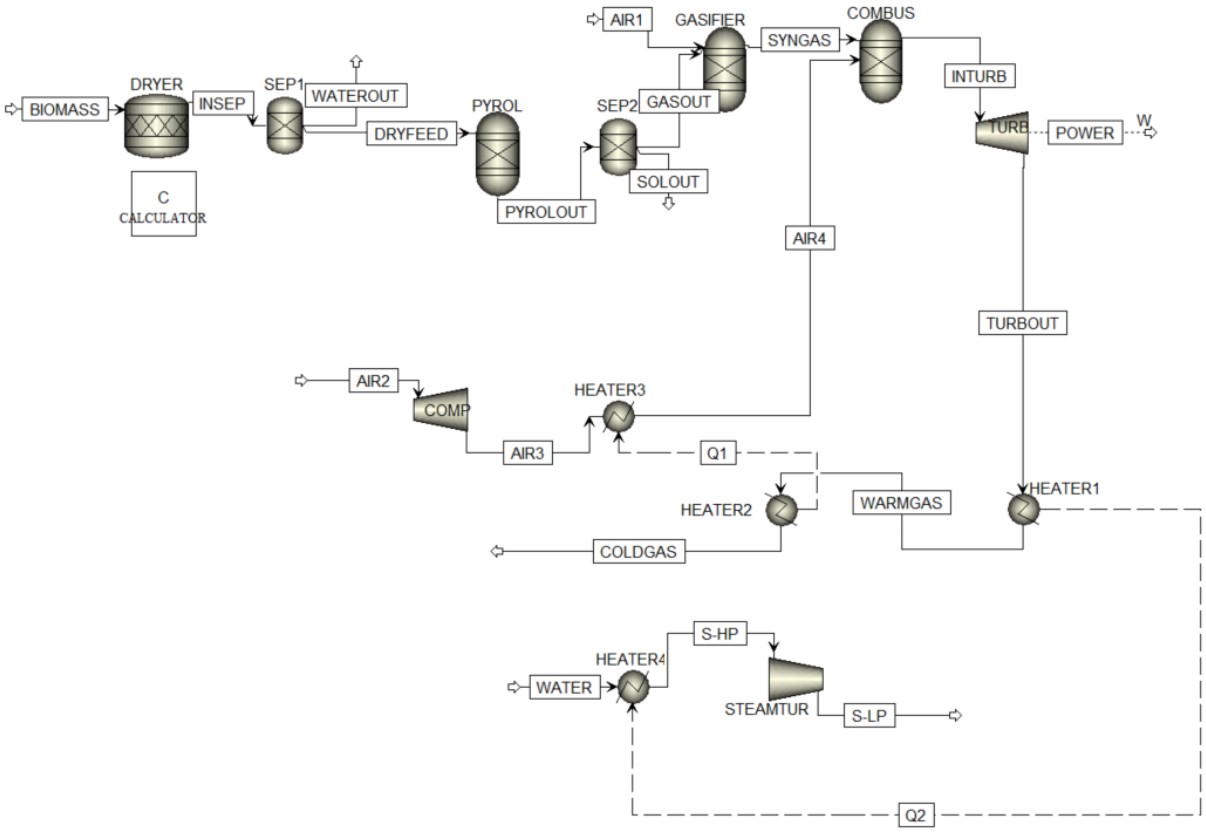


Figure 3-2. Flow chart of the advanced simulation model for gasification by using Aspen Plus

3.2.2 Case study

An overview of different Icelandic municipalities is shown in Figure 3.3. West (A), Suðurnes (B), South (C), Capital area (D), East (E), Northeast (F), Eyjafjörður (G), Northwest (H) and Westfjords (I), [1]. Western Iceland consists of 10 municipalities with a total of 15 thousand occupants in 2010. Suðurnes contains 5 municipalities with a total of 21 thousand inhabitants in 2010. The Capital Area covers 8 municipalities with 200 thousand residents. Southern Iceland consists of 14 municipalities with a total of 23 thousand inhabitants. East contains 9 municipalities with a total of 12 thousand inhabitants. Northeast covers 6 municipalities with a total of 5 thousand occupants. Eyjafjörður includes 8 municipalities with 24 thousand residents. There are 8 municipalities in Northwest with a total population of 7500 and finally Westfjords contains 9 municipalities with 7 thousand inhabitants in 2010 [1].

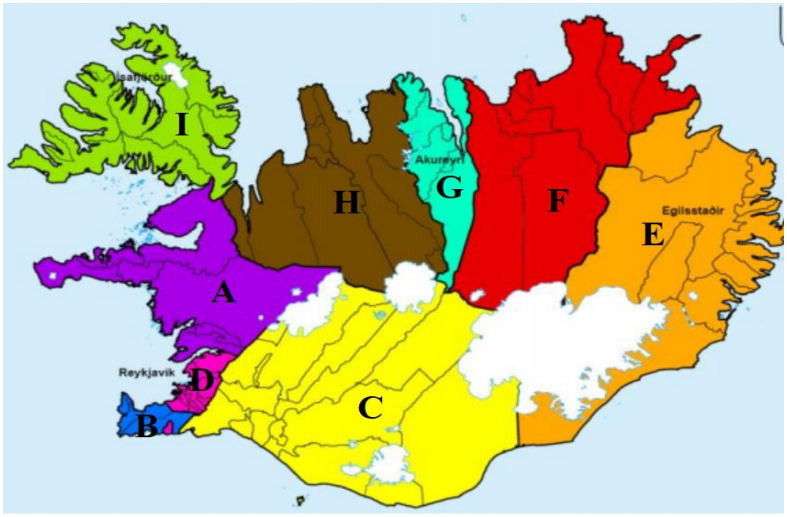


Figure 3-3. The overview of different Icelandic municipalities

Organic waste from households, industry and services is a valuable source for biofuels production in Iceland. The Icelandic Environmental Agency set up a National plan to reduce the amount of organic wastes that are landfilled or incinerated over the years. A general estimation shows that approximately 60% of the total waste is organic material of which 70% is obtained from industry and services and 30% is from the household sector [1].

Categories of organic waste from household, industry and services are defined as, garden waste, timber and wood waste, mixed paper waste, fish waste, meat and slaughter waste, kitchen waste, and waste bio oil. Among these organic wastes, garden waste, timber and wood waste, and mixed paper waste are the main wastes that can be fed to a gasifier. The main sources of mixed paper waste that are suitable for gasification are newspapers, magazines and packaging waste. In addition, the main sources of timber waste are timber from construction, demolition work, packaging waste and pallets. Garden waste can be also defined as grass, branches and other garden waste.

Figure 4.8 shows the total amount of these kinds of organic waste for various Icelandic parts in 2020. As is shown in Figure 3.4, the Capital area is the dominant region in all waste production with more than 60% of the Iceland population in this area. However, the Capital area occupies just 1% of total area. This is because of the lack of development and urbanization in this location, lack/ shortage of proper climate and geographical conditions in other places and transportation issues [5]. Moreover, the total amount of paper, timber and garden wastes in Iceland in 2015 have been calculated as approximately 37, 40 and 16 thousand tons, respectively, and they have been estimated to increase to about 47, 49 and 20 thousand tons by 2030 assuming 0.8%, 0.6% and 0.6% growth rate per capita, respectively.

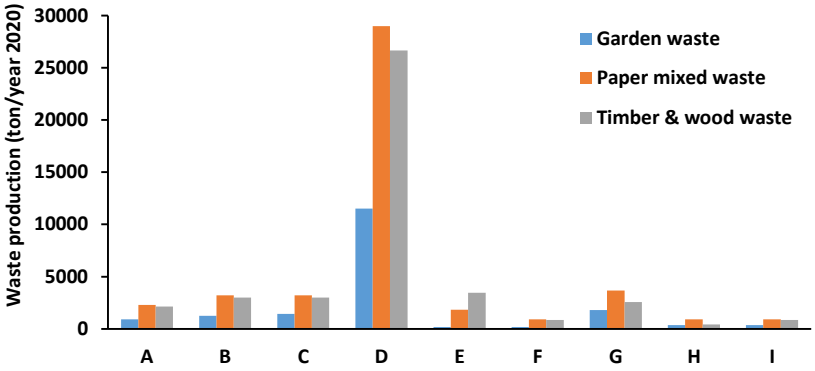


Figure 3-4. The amount of various wastes production in different Icelandic municipalities in 2020

3.3 Environmental assessment

It is totally true that collecting and disposal of wastes have so many advantageous for human health and well-being, environmental preservation and sustainability that can be said these benefits are the main/direct impacts of waste disposal. However, improper management of wastes poses serious threats and damage to environment and human health. Landfilling and incineration have been the only methods of disposal of solid wastes in many countries like Iceland, while most landfill sites have been open dumping areas, which pose serious environmental and social threats and incinerators release much pollutions to the atmosphere that these losses can be considered as the alternative/indirect impacts of waste disposal. Therefore, it is really important to apply technologies for waste disposal that have the minimum environmental (indirect) impacts.

In this part an environmental assessment from the integrated waste biomass gasification with power unit is carried out to find that the considered system could be satisfied from environmental viewpoint and then the results of integrated waste gasification and power system is compared with waste incineration as a conventional and currently running system in Iceland to find how much reduction in pollution will be happened when gasification is used for waste disposal. The results of this part have been published in Paper VI and X.

The system boundary considered for environmental assessment includes all the process steps from the initial resources to the end products (Figure 3.5).

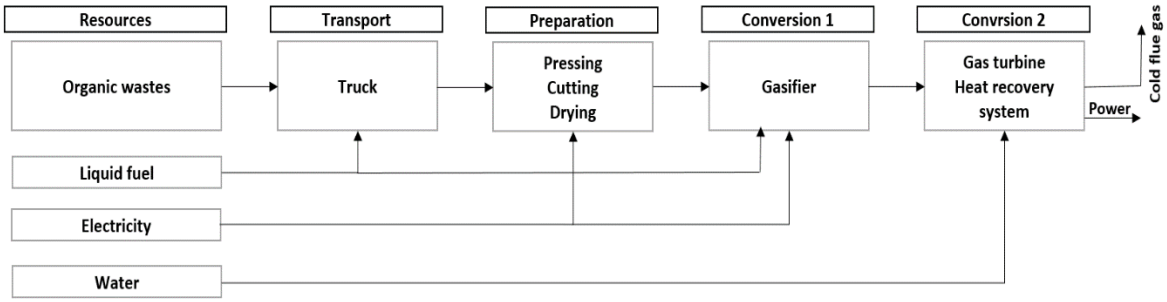


Figure 3-5. System boundaries, considered for environmental assessment (technologies and associated inputs, energy and material)

In the resource step, organic wastes are the main input resources. Energy and water are also considered as accessory inputs. Diesel fuel used by trucks for transportation and electricity consumed for driving force and heat generation in process units are also considered. The electricity production in Iceland is derived from geothermal and hydropower making the main source of clean energy. Waste is transferred from the waste fields to pre-processing units that are located next to gasification and power production plants. The gasification process consists of drying, pyrolysis, combustion and gasification [137]. The produced syngas from the gasifier enters a combustion chamber followed by a gas turbine. The combination of these two modules represents the behavior of a combustion engine where the reaction with air occurs. The thermal content of the gas is obtained as the heat of combustion is removed and used to convert boiler feed water to high pressure steam. The generated steam finally drives a steam turbine, producing additional power. Key assumptions regarding inputs for each process are listed in Table 3.2 [5, 34, 133, 134, 138, 139]. Environmental assessment can be defined as identifying and estimating of the environmental impacts of existing and proposed systems to mitigate the relevant negative effects prior to making decisions [140]. The impact categories in this work are global warming (GWP), acidification (AP) and eutrophication (EP) potentials; these impact categories were selected because they are the main indictors that cover most important indirect environmental impacts of gasifier used for waste disposal [34, 141]. GWP concentrates on greenhouse gas emissions (GHG) and their impact on global warming. GHGs are atmospheric gas compounds (CO_2, CH_4 and NO_2) that trap heat through emitting radiation in the atmosphere. The increase in the amount of these gases results in keeping the surface of the earth warmer by absorption of the sun light that passes through the atmosphere freely [138, 140]. Moreover, both of acidification and eutrophication accelerate climate change, acidification reduces the carbon uptake of water bodies, and eutrophication darkens water bodies and leads to less reflectivity, and reduces the carbon storages in the bottom sediments. Acidification is also an environmental problem caused by acidified rivers/streams and soil due to anthropogenic air pollutants of SO_2, NH_3, H_2SO_4, H_2S, HCL, SO_3 and NO_x. These kinds of emissions come down to the ground as acid rain or snow to be absorbed into lakes, rivers, and soil. As a result, surface water, ground water and soil are acidified in ways that cause devastation of forests and many shelled animals. Eutrophication is also a phenomenon in which inland waters are heavily loaded with excess nutrients due to chemical fertilizers or discharged wastewater, triggering rapid

algal growth and red tides. The major substances with impacts on eutrophication were found to be NO_x, NH_3, N_2, and NO_3 in the case of air [6].

Table 3-2. List of some assumption for environmental assessment regarding inputs for each step

Step	Unit	Amount	Comment	Ref
Resources				
Waste input	ton	1		
Transport				
Distance	km	100	Distance from fields to energy conversion plants	
Diesel fuel	L/km.ton	0,06		[5, 138, 139]
Preparation				
Electricity for pressing & cutting	kWh/ton	5,48		[34]
Conversion 1				
Unit Fuel oil	L/ton	0,2	It is for start-up of the gasifier	[34]
Unit Electricity	kWh/ton	83		[34]
Conversion 2				
Isentropic efficiency of compressor	%	90		[34, 134]
Mechanical efficiency of compressor	%	99		[34, 134]
Isentropic efficiency of gas turbine	%	90		[34, 133]
Isentropic efficiency of steam turbine	%	92		[34, 133]

The impact assessment methods employed in this work are based on IPCC 2007 and other research works in this field [34, 141]. The GWP, AP and EP factors for key input in to the system and their factors for different emitted substances are summarized in Table 3.3 [5, 34, 139] and Table 3.4 [142], respectively.

Table 3-3. GWP, AP and EP factors for different inputs

Input	Unit	GWP factor ($kgCO_{2eq}$/unit)	AP factor (gSO_{2eq}/unit)	EP factor (gNO_{3eq}/unit)
Electricity generated from geothermal	kWh	0.058 [5]	1.95 [5]	2.8 [5]
Transport by truck	ton.km	0.3 [5, 139]	2.1 [34]	4.2 [34]
Liquid fuel used in gasifier	lit	2.76 [34]	10.5 [34]	21[34]

Table 3-4. GWP, AP and EP factors for different emitted substances

	GWP factor ($kgCO_{2eq}/kg_{substance}$)	**AP factor ($kgSO_{2eq}/kg_{substance}$)**	**EP factor ($kgNO_{3eq}/kg_{substance}$)**
CO_2	1		
CH_4	25		
N_2			0.042
O_2			
S			
SO_2		1	
NH_3		1.88	3.64
NO		1.07	0.02
N_2O	298		
CL_2			
HCL		0.88	
NO_2		0.7	0.013
H_2SO_4		0.65	
NO_3			1

3.4 Techno-economic assessment

In this part a techno-economic assessment from the integrated waste biomass gasification with power unit is carried out to find that the considered system could be satisfied from economic viewpoint and then the results of this part have been published in Paper VIII and IX.

The studied system for techno-economic assessment includes the process steps from resources to the end product (Figure 3.6).

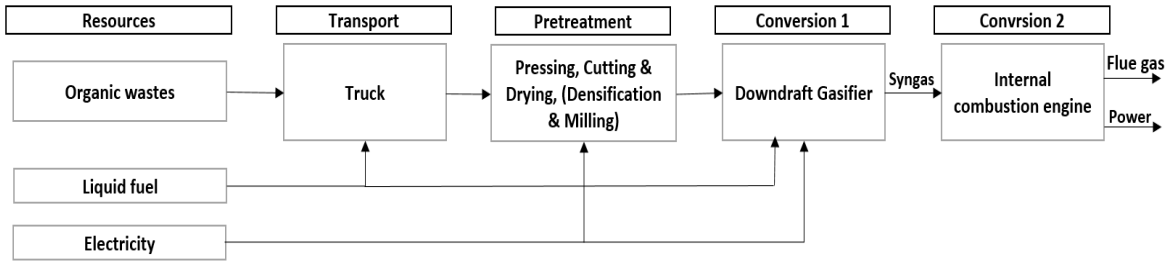


Figure 3-6. System boundaries, technologies, energy and material streams for techno-economic assessment

As mentioned in the Section of environmental assessment, the organic waste is the significant resource entering to the system, liquid fuel and electricity are also the accessory inputs. Biowastes is transferred from the waste fields to pre-treatment part that is next to

gasification and electricity generation unit. Then the product syngas enters in internal combustion engine that is modelled as a combustion chamber followed by a gas turbine. The combination of these two modules represents the behaviour of a combustion engine where the reaction with air occurs [133, 143]. The inputs values and key assumptions are shown in Table 3.5, the main values of the downdraft gasifiers characteristics, operational parameters and the flue gas composition derived from the waste biomass gasification simulation model [29] have also listed in Table 3.5.

Table 3-5. Input values, assumptions, gasifier characteristics, operational parameters and flue gas composition

Step	**Unit**	**Amount**	**Comment**
Transport			
Distance	km	100	Distance from fields to energy conversion plants
Diesel fuel	L/km. $ton_{T\&WW}$	0,06	
Preparation			
Electricity for pressing & cutting	kWh/ $ton_{T\&WW}$	5,48	
Conversion 1			
Type of gasifier			Downdraft fixed bed (autothermal)
Gasification agent			air
Gasification pressure	kPa	101.3	
Gasification temperature	˚C	800	
Equivalence Ratio (ER)	-	0,25	
Specific air mass flow rate consumption	$kg/kg_{T\&WW}$	1,8	
Unit Fuel oil consumption	L/ $ton_{T\&WW}$	0,2	It is for start-up of the gasifier. $ton_{T\&WW}$ refers to ampunt of T&WW that enters to gasifier after pre-process step
Unit Electricity consumption	$kWh/ton_{T\&WW}$	83	$ton_{T\&WW}$ refers to ampunt of T&WW that enters to gasifier after pre-process step
Conversion 2			
Isentropic efficiency of compressor	%	90	
Mechanical efficiency of compressor	%	99	

Net produced power	kWh/yr	2820,8 MT&WW (kg/hr) + 2293,3	as functional of mass flow rate of biomass
Specific mass flow rate of flue gas exited from gas turbine	$kg/kg_{T\&WW}$		
CO		0,226	
CO2		1,62	
H2		0,00247	
H2O		0,645	
CH4		0	
N2		5,316	
O2		0,082	
S		0	
SO2		0,0013	
H2S		0	
NH3		0	
NO		0,049	
N2O		0	
CL2		0	
HCL		0	
NO2		0,000037	
H2SO4		0	
NO3		0	

In this economic analysis, all prices are expressed in K€ (kilo-euro). Three scenarios were considered based on different interest rates: 8% in Scenario 1, 10% in Scenario 2 and 13% in Scenario 3. These are based on interest rates considered for European energy projects [144, 145]. A computer program has been developed to investigate these scenarios for specific case study. The model is able to evaluate the economic performance of each one. Cash flow analysis, total cost, Net Present Value (NPV) and Discounted Payback Period (DPP) are standardized financial indicators to assess the profitability of projects. A project is an economically attractive while it has the lowest DPP and the NPV higher than zero. NPV is the difference between the present value of cash inflows and the present value of cash outflows over a period of time and it is calculated based on Equation (7) [44, 45, 113]:

$$NPV = \sum_{n=1}^{t} \frac{CF_n}{(1+r)^n} - C_c \tag{7}$$

where CF_n is the annual cash flow, being the difference between Revenues (R) and Expenditures (E), Operation and Maintenance Costs ($C_{O\&M}$), r is the discount rate (8%, 10% and 13% for Scenario 1, 2 and 3, respectively), C_c is the total capital costs of investment and t is the lifetime of the investment (15 years). DPP gives the number of years

to break even from undertaking the initial expenditure, by discounting future cash flows and recognizing the time value of money and it is calculated according to Equation (8) [44, 45]:

$$DPP = \frac{LN(\frac{1}{1-\frac{C_c \times r}{CF}})}{LN(1+r)} \quad (8)$$

The periodic cash flow, with all the revenues and expenditures, is calculated by considering the incomes from the generated electricity, and the credits for the Waste Treatment Bill (WTB) [146]. The expenditures also include the C_c and $C_{O\&M}$. C_c is divided into three categories: hardware price (C_g), installation cost (25% of C_g) and engineering costs, the engineering costs includes engineering and design (13% of C_g), purchasing & construction (14% of C_g), fuel handling/preparation (9% of C_g) and electrical/balance of plant (6% of C_g) [144, 145]. C_g is the price of a gasifier system on the basis of various capacities. In this work, we considered 0.75, 1.5, 2, 5, 10, 20, 50, 100, 200, 300, 400 and 500 kW for the small-scale existing gasifiers capacities and extracted their prices from various companies (Figure 3.7) [147-152].

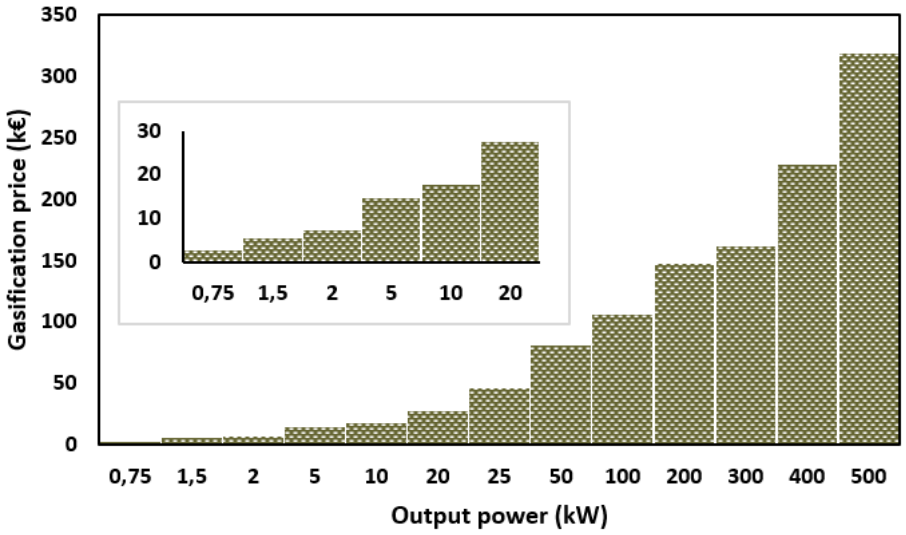


Figure 3-7. The small-scale existing gasifiers capacities and extracted their prices from various companies

The whole yearly $C_{O\&M}$ can be determined by the sum of the costs for the maintenance cost (2% of C_c), insurance and tax (2% of C_c), waste disposal (15% of C_c), electricity cost, liquid fuel cost and personnel cost. Electricity costs are calculated based on electricity consumers and liquid fuel costs are estimated for fuel consumers with 7000 hr/year of plant availability [144, 145]. The unitary cost of electrical and fuel energies supplied in Iceland

are equal to 0.03 $/kWh and 1.08 $/lit (0.91 €/$ as conversion rate) [5]. Personnel cost includes annual labour, cost. A total of two employees were assumed for plant operation management (1 person/shift and 2 shifts/day), with a yearly cost of 60,000 €/year per person in Iceland.

In relation to revenues, the selling price of electricity to normal households and small businesses in Iceland is about 124.69 $/MWh [153]. Hence, the sale price of the generated electricity based on waste gasification was considered at 109.89 $/MWh (100 €/MWh) in our work. Moreover, The Icelandic municipalities pay a fee (WTB) by weight, to the private companies, for the collection and disposal the MSW in sanitary landfills. The WTB for collection and disposal of the MSW varies from 90-170 €/ton through over Iceland. The highest amount is related to Vestmannaeyjar, an archipelago off Iceland's south coast with 111 km distance from Reykjavik (the Capital of Iceland). All produced waste in Vestmannaeyjar need to be collected and transferred to other Icelandic municipalities for disposal. Hence, WTB for this area is in the top due to geographical conditions and expensive transportation. In this work a mean value of 130 €/ton is used.

4 Results and discussions

This Chapter includes 4 sections containing results for primary model, advanced model, environmental assessment and techno-economic assessment. Responses to RQ3, RQ4, RQ5 and RQ6 can be found in Sections of 4.1, 4.2, 4.3 and 4.4, respectively. Response to RQ1 has been also brought in Section 3.2.2 Case study. It is worth to say that response to RQ2 was presented in Section 2.2 Biomass gasification models.

4.1 Primary model

4.1.1 Validation

For validating the primary model, the syngas composition obtained from ASPEN simulations were compared with the experimental results of Jayah et al [154]. In their work, rubber wood was used as feedstock in a down draft gasifier operated at atmospheric pressure and gasification temperature of 900 ˚C. Six different air to fuel mass flow rate ratios (AFRs) were considered and the comparisons of CO, H_2, CO_2 and N_2 concentrations are shown in Figure 4.1. The deviation of the model results from experimental values is quantified by using statistical parameter RMS. RMS measures how much error there is between two data sets (experimental data and modeling values). Its value close to zero indicates lower error and more reliable model in prediction of results. The maximum RMS error of 1.8 is gained when six sets of experimental data are compared with the corresponding model values for syngas composition. The obtained RMS in this work is good and acceptable because it is not far from zero and also lower than other works in this field. For example the latest developed model by Rupesh et al. [82] has RMS of 2.8 in comparison with experimental data for product gas compositions.

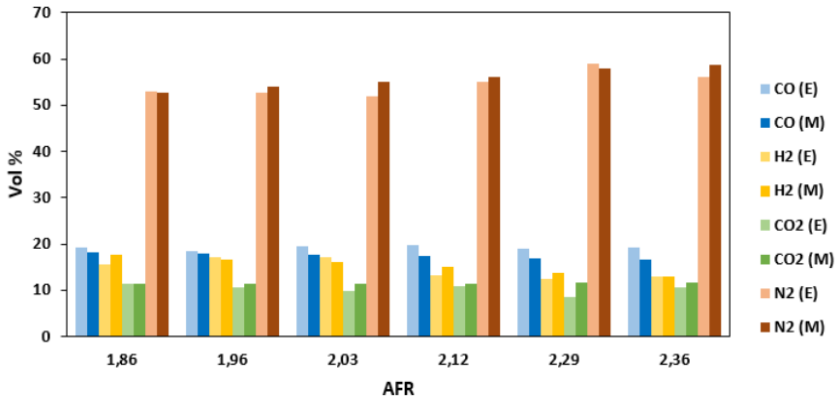


Figure 4-1. Comparison of CO, H2, CO_2 and N_2 concentrations between the developed model (M) and experimental measurements (E)

4.1.2 Performance analysis

In this part, the developed model for waste biomass gasification has been used to investigate the gasification performance of three different waste feedstocks: sawdust, wood chips and mixed paper waste. The biomass characteristics used to describe the feedstocks are given in Table 4.1. The effect of gasifier temperature and equivalence ration (ER) on syngas composition, syngas yield, lower heating value (LHV) of produced gas and cold gas efficiency (CGE) has been investigated. Syngas yield in this model is the volume of total product gas from the gasification per unit weight of fuel in normal conditions (Nm^3 kg $fuel^{-1}$). The lower heating value of product gas is calculated as [80, 155]:

$$LHV_{syngas}(kj/Nm^3) = 4.2 \times (30 \times y_{CO} + 25.7 \times y_{H_2} + 85.4 \times y_{CH_4}) \quad (9)$$

where y is the mole fraction of gas pieces in the syngas (dry basis).

The CGE is also calculated by using Equation (10) [80, 156]:

$$CGE(\%) = \frac{G_P \times LHV_{syngas}}{HHV_{fuel}} \times 100 \quad (10)$$

where G_P is the syngas yield that is the volume of total product gas from the gasification per unit weight of fuel in normal conditions (Nm^3 kg fuel-1). HHV_{fuel} is the higher heating value of fuel (MJ kg fuel-1) [157].

$$HHV_{fuel}(Mj/kg) = 0.312 \times (FC) + 0.1534 \times (VM) \quad (11)$$

According to Equation (11), heating value is a function of weight fractions of fixed carbon and volatile matter in the dry and ash-free conditions.

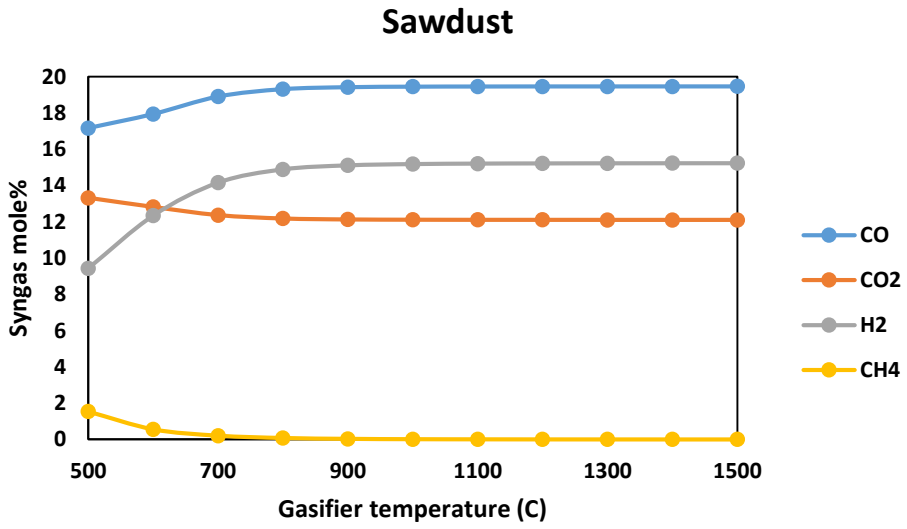
Table 4-1. Ultimate and proximate analysis feedstocks

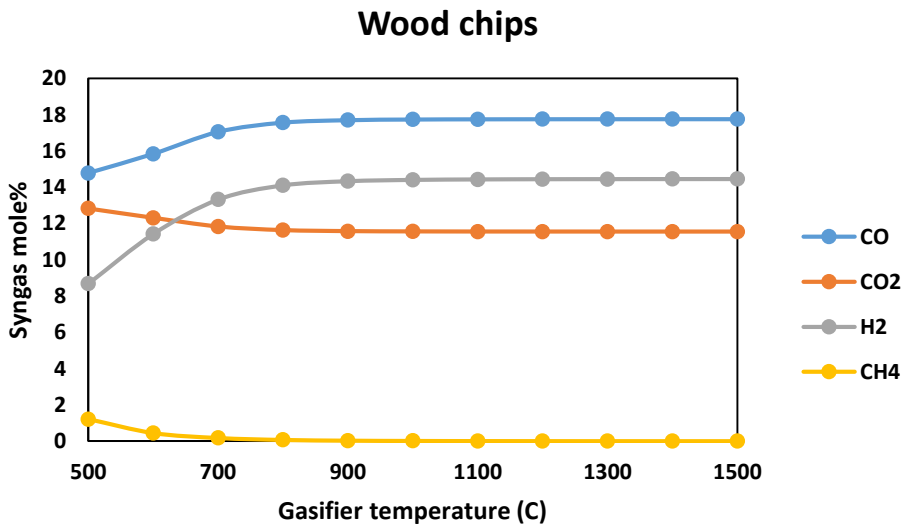
Feedstocks	Sawdust	Wood chip	Mixed paper waste
Proximate analysis			
Proximate analysis (wt%)			
Moisture	7	20	8.8
Volatile matter (VM)	81.72	80	84.2
Fixed carbon (FC)	17.2	18.84	7.5
Ash	1.08	1.16	8.3
Ultimate analysis			
Elemental analysis (wt%- dry basis)			
C	46.46	51.19	47.96
H	5.82	6.08	6.60
N	0.19	0.2	0.18
O	46.45	41.37	36.96

4.1.2.1 Effect of temperature on syngas composition

The effect of gasifier temperature on syngas mole fractions for three feedstocks was examined in the window of 500-1500 ˚C, while all the remaining operating conditions were fixed. As shown in Figure 4.2, at very low temperature of 500 ˚C the existing carbon in the biomass is not used completely, so the syngas production would not be in a good rate. In such a low temperature, unburned carbon and methane will remain in syngas while by increasing temperature more carbon is oxidized and converted to carbon monoxide in accordance with partial combustion reaction (R2). Methane is also transferred into hydrogen by reverse methanation reaction (R5). Moreover, at high temperature, water gas reaction (R4) goes toward the production of both carbon monoxide and hydrogen. Hence, increasing the gasifier temperature favors hydrogen and carbon monoxide production, leads to the improvement of heating value of syngas (based on Equation (9)). However, at a specific temperature, yield of H_2 and CO reach to an approximately fixed points that this point can be the optimum gasifier temperature for each waste. The optimum operating temperature of the down draft gasifier for sawdust, wood chips and paper wastes are 900, 1000 and 1000 ˚C, respectively. Methane production also decreases sharply at temperatures above 600 ˚C

for three wastes. For both sawdust and wood chips wastes, mole fraction of CO is higher than H_2 mole fraction but general behavior is not the same for paper waste. According to the elemental analysis of feedstocks, mixed paper waste has the highest hydrogen and the lowest oxygen among the others, consequently the product gas from paper gasification includes lower CO but higher H_2 in comparison other wastes.





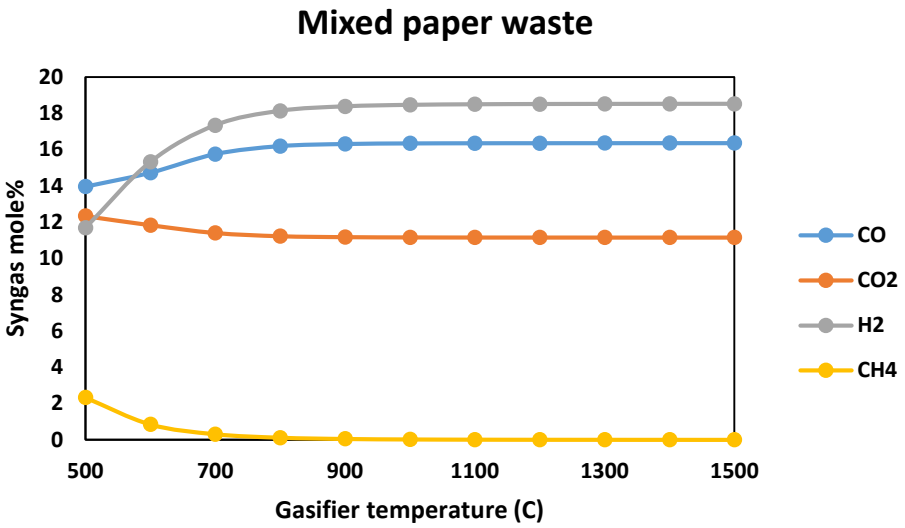


Figure 4-2. Effect of temperature on syngas mole fraction (dry basis)

4.1.2.2 Effect of ER on syngas composition

Equivalence Ratio (ER) is an important index for showing the role of oxidizing agent and it is defined as the ratio of the amount of actual air supplied to the gasifier to the stoichiometric air. At low ER, biomass reactions will approach to the pyrolysis, whereas at a high ER the excess amount of oxygen oxidizes the fuel completely and causes biomass combustion; then the production of syngas declines. Hence, it is important to find the appropriate range of ER for biomass gasification that has been studied in this work. In this case, the ER in the gasifier was varied from 0.1-0.7 and its influence on the syngas compositions were shown in Figure 4.3 for three wastes. The H_2 mole fraction decreases with increasing ER, regardless of which biomass is used as the feedstock. Similar to H_2 formation, the mole fraction of CO also decreases with increasing ER but an opposite trend for CO_2 is exhibited. This is due to when ER rises, more oxygen is supplied for biomass reactions, so fuel goes toward the full combustion. Sawdust has highest mole fraction of carbon monoxide and hydrogen in syngas (0.28 and 0.38, respectively). Conversely, the gasification of mixed paper waste gives the lowest mole fraction of CO (0.22). Finally, as shown in Figure 4.3 the optimum ER lies between 0.2-0.35 for three wastes (till mole fractions of carbon monoxide and hydrogen are higher than 20%).

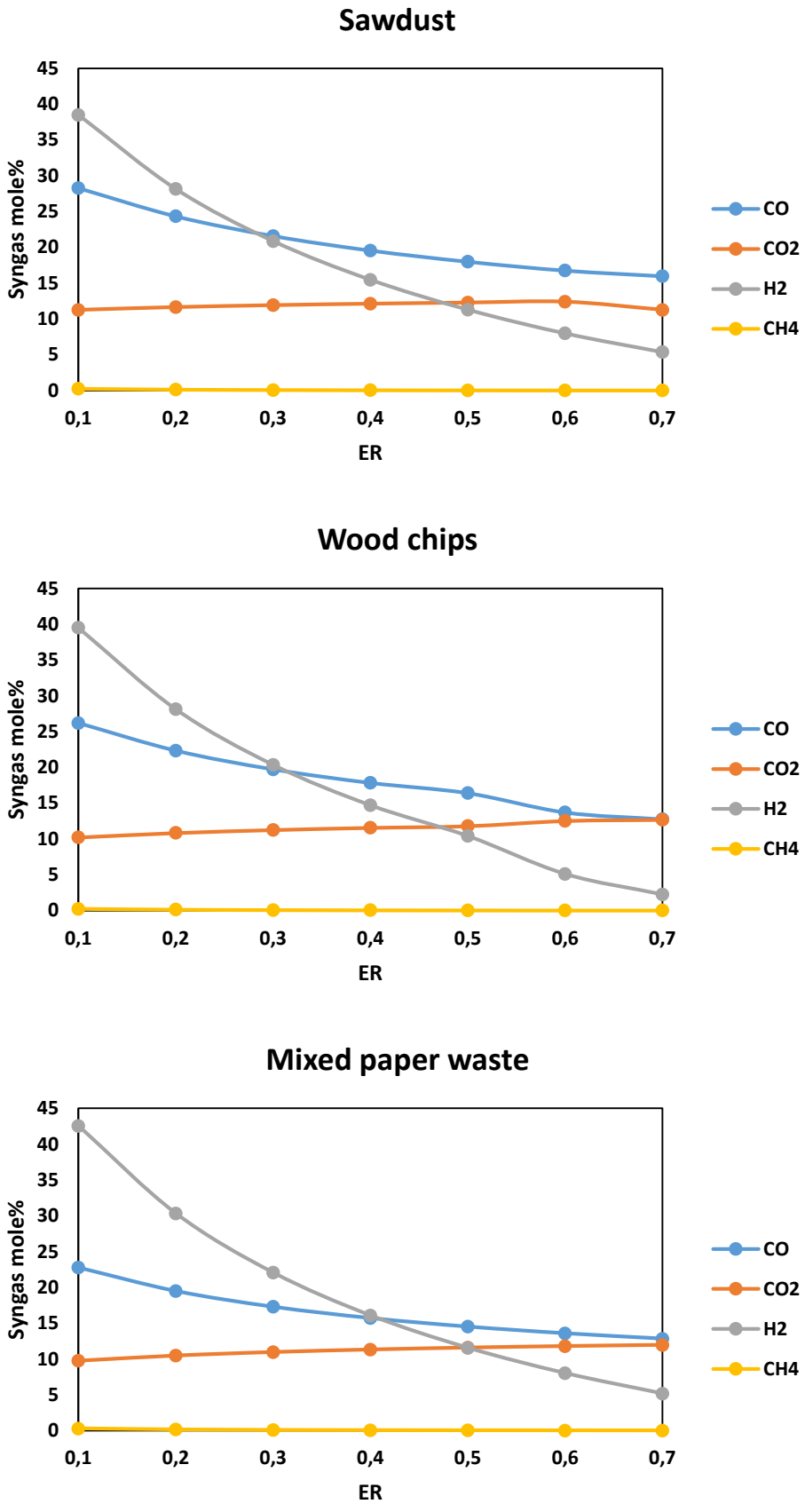


Figure 4-3. Effect of ER on syngas mole fraction (dry basis)

4.1.2.3 Effect of temperature and ER on syngas yield

The effect of the gasifier temperature on the syngas yield is illustrated on Figure 4.4(a). When the operating temperature of gasifier is increased from 500-900 ˚C, the syngas yield is increased 4.6% for sawdust and wood chips and 5.4% for mixed paper waste and then reach to approximately fixed points. It can be explained by increasing gasifier temperature, the unburned carbon is converted into carbon monoxide and through the reverse methanation reaction, methane is converted into hydrogen. Finally, mole fractions of components attain to the constant amounts that cause nearly constant values for syngas yield. Figure 4.4(a) depicts that the syngas yield for wood chips gasification is higher than other wastes, because syngas production from gasification of wood chips waste has highest carbon monoxide and hydrogen due to high percentage of carbon and hydrogen in wood chips biomass (as shown in Table 4.2).

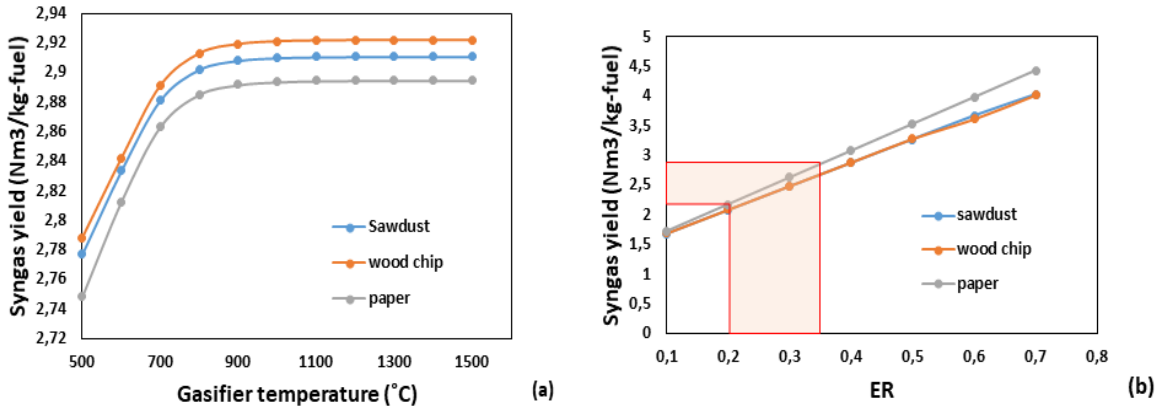


Figure 4-4. (a), Effect of temperature on syngas yield, (b), Effect of ER on syngas yield

The variation of syngas yield for three wastes by varying ER is shown in Figure 4.4(b). The syngas yield from the gasification of paper waste is higher than that of wood chip and sawdust wastes averagely 7.3%. As ER increases from 0.1 to 0.7, syngas yield continuously increases because more oxygen is available for biomass reactions at high ER but so high syngas yield does not mean high gasification performance. Because as it was explained in section 4.2, with access to more oxygen, the fuel is oxidized completely and causes biomass combustion; then the production of CO and H_2 decline and CO_2 production increases. In the optimum range of ER, syngas yield values for sawdust, wood chips and paper wastes are in the span of 2.08-3.00 Nm^3 kg $fuel^{-1}$.

4.1.2.4 Effect of temperature and ER on LHV

Figure 4.5(a) shows the lower heating value of syngas as a function of temperature. The increase in temperature of the gasification zone at fixed AFR of 2.03 results in an increase in the LHV of the syngas till a specific temperature that is called optimum temperature. LHV values for sawdust, wood chips and mixed paper wastes at optimum temperatures (900, 1000 and 1100 ˚C, respectively) are about 4.09, 3.79 and 4.06 MJ Nm^{-3}, respectively. Wood chip

shows lowest heating value among the three wastes due to relatively lower dry basis mole fraction of carbon monoxide and hydrogen in the syngas. The production of carbon monoxide and hydrogen is dependent on the biomass composition and it is clear from the composition of feedstocks provided in Table 4.3 that although wood chip has highest percentage of carbon, it includes so high amount of moisture. Moisture content indirectly effects on LHV of syngas. Increasing moisture content strongly degrades the syngas LHV. As a consequence of much higher moisture content in the fuel, the percentage of carbon and hydrogen in wet basis decrease then leads to lower production of carbon monoxide and hydrogen in the syngas.

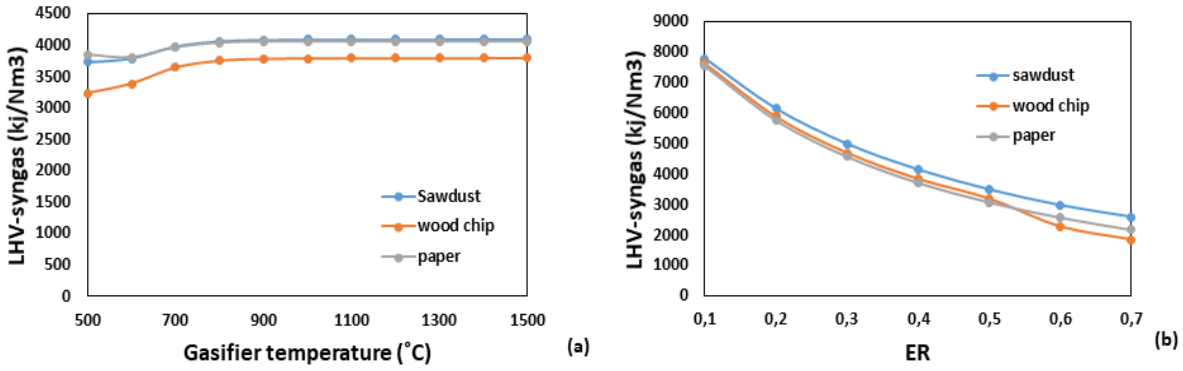


Figure 4-5. (a) Effect of temperature on syngas LHV, (b), Effect of ER on syngas LHV

The sensitivity of ER over the LHV of the product syngas at the fixed gasifier temperature of 900 ˚C for three waste biomasses are shown in Figure 4.5(b). By increasing ER, the production of carbon monoxide and hydrogen in syngas decrease due to complete combustion of fuel, so the heating value of the syngas decreases. As a whole, the LHV of the product gas depends strongly on ER and it is in the range of 4.15 and 6.147 MJ Nm^{-3} In the optimum range of ER. On the other hand, the effect of feedstock on LHV is slight.

4.1.2.5 Effect of temperature and ER on CGE

Cold gas efficiency is the most crucial parameter that practically indicates the economic efficiency of the gasifier. Accordance to equation (2), CGE is dependent on different parameters of syngas yield, HHV of fuel and LHV of syngas, but it eventually depends on the amount of carbon monoxide, hydrogen and methane in the product syngas. The composition of syngas is also controlled by temperature and ER hence they are the important parameters for evaluating of CGE. In our model temperature has been varied from 500-1500 ˚C and the corresponding CGE is calculated. The results have been depicted in Figure 4.6(a). Mixed paper waste shows highest CGE (70.6%) at temperature of 1000 ˚C while for sawdust CGE is maximum around 65,8% and wood chips shows lowest CGE (60%) among the three wastes. Figure 4.6(b) shows that increasing ER reduces the value of CGE, stemming from the reduction of LHV (Figure 4.5(b)). For the three waste biomasses, the amount of CGE is under 60% as long as ER is more than 0.4. It follows that ER should be controlled below 0.4.

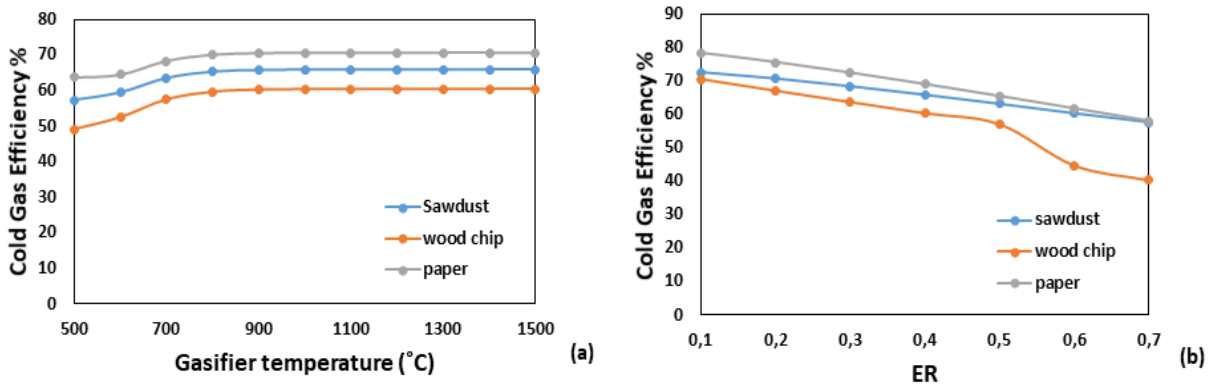


Figure 4-6. (a), Effect of temperature on CGE, (b), Effect of ER on CGE

4.2 Advanced model

The main objective of this part is to analyze the performance of the biomass gasification integrated with the power production unit based on the simulation model developed by using ASPEN Plus. The case study assesses power production in Iceland from 1ton of 3 different Icelandic organic wastes: garden waste, timber and wood waste, and paper mixed waste [5], as it was mentioned in Section 3.2.2. The elemental and gross compositions of these feedstocks were gathered in Table 4.2 [158, 159]. Then, as a sensitivity analysis, we examine the effect of operating parameters like temperature and equivalence ratio (ER) to know where the overall system is optimal to reach the maximum electrical efficiency.

As it mentioned above, in this part, the developed model for waste biomass gasification has been used to investigate the gasification performance of garden, timber and wood, and paper mixed wastes in Iceland. The goal is to find the optimal operating conditions in order to produce the highest power efficiency. The important operating variables that affect power performance are the gasifier temperature and the equivalence ratio (ER). The effect of temperature and ER on power efficiency of the gasifier system is shown in Figures 4.9 and 4.10, respectively. The power efficiency is the index of the power generated from the system compared to the original energy contained in the biomass feed and is defined by [128]:

$$\eta_{power} = \frac{W_{gas\ turbine} + W_{steam\ turbine} - W_{compressor}}{M_{biomass} \times LHV_{biomass}} \quad (12)$$

The sensitivity results in Figures 4.9 and 4.10 are studied at standard conditions of 1 ton input of feedstock, a 2.5 air to biomass ratio and a gasifier temperature in the window of 500-1500 ˚C. As seen in Fig. 5, all wastes show a similar increasing behavior as the temperature rises. As it mentioned in Section 4.1.2.1, since the gasifier temperature increases, H_2 and CO flow rates increase, too. However, CO_2 and CH_4 flow rates decrease with the increase in the temperature. Growing of CO and H_2 flow rates in the range of 500

Table 4-2. Ultimate and proximate analysis of feedstocks that are used in simulation of feedstocks in ASPEN Plus

	Garden waste	**Timber & wood waste**	**Paper mixed waste**
Proximate analysis			
Proximate analysis (wt%)			
Moisture	50	5.01	10.24
Volatile matter (VM)	84.5	93.06	84.60
Fixed carbon (FC)	14.5	6.38	9.40
Ash	1	0.56	6
Ultimate analysis			
Elemental analysis (wt%- dry basis)			
C	50.12	56,8	43,41
H	6.40	7,28	5,82
N	0.14	0,18	0,25
Cl	0	0,82	0
S	0.08	0,07	0,2
O	42.26	34,29	44,32

to 700 °C is because of the combined effect of boudouard, steam methane reforming and water-gas reaction. These are endothermic reactions in nature, hence they are favored with higher temperature. Moreover, reduction in CO_2 and CH_4 flow rates with increasing temperature is due to the exothermic nature of water gas shift and methanation reaction, making them unfavorable at higher temperatures.

By increasing the gasification temperature, water gas and steam methane reforming reactions contributed majorly to H_2 production, but steam methane reforming reaction is limited due to the absence of CH_4 as the main reactant at a higher temperature. As a whole, it can be concluded that water gas shift reaction mainly controls the H_2 production. In addition, the reduction in CO_2 flow rate by increasing the temperature can be associated with the boudouard reaction which utilizes CO_2 to produce CO and being endothermic in nature that is favored at higher temperatures. Hence, increasing the gasifier temperature favors hydrogen and carbon monoxide production, leading to high LHV syngas enter to the combustion chamber and resulting high temperature gases entering the turbine. Raising the turbine inlet temperature increases output power from the gas turbine, as well as the steam turbine, because more steam is produced through the heat recovery from the high temperature flue gas. However, at a specific range of temperature, power efficiency increases in a gradual way such that this span can be the optimum gasifier temperature for each waste. The optimum operating temperature of the down draft gasifier for the three studied wastes was 900-1000 ˚C.

Moreover, Figure 4.9 shows timber and wood waste has dominant statues for power efficiency among the three wastes due to relatively higher net power production through the system. The amount of power production is dependent on the biomass composition and it is clear from the composition of feedstocks provided in Table 4.2 shows timber and wood has the highest percentage of carbon and hydrogen and lowest amount of moisture. Hence, this kind of waste would be the best option to be fed to a gasifier and power production plant. However, garden waste with the highest moisture content of 50% has the lowest potential for power production. Moisture content indirectly effects output power as a higher moisture content in the fuel leads to a decrease in the percentage of carbon and hydrogen in a wet basis leading to a lower production of carbon monoxide and hydrogen as well as lower LHV.

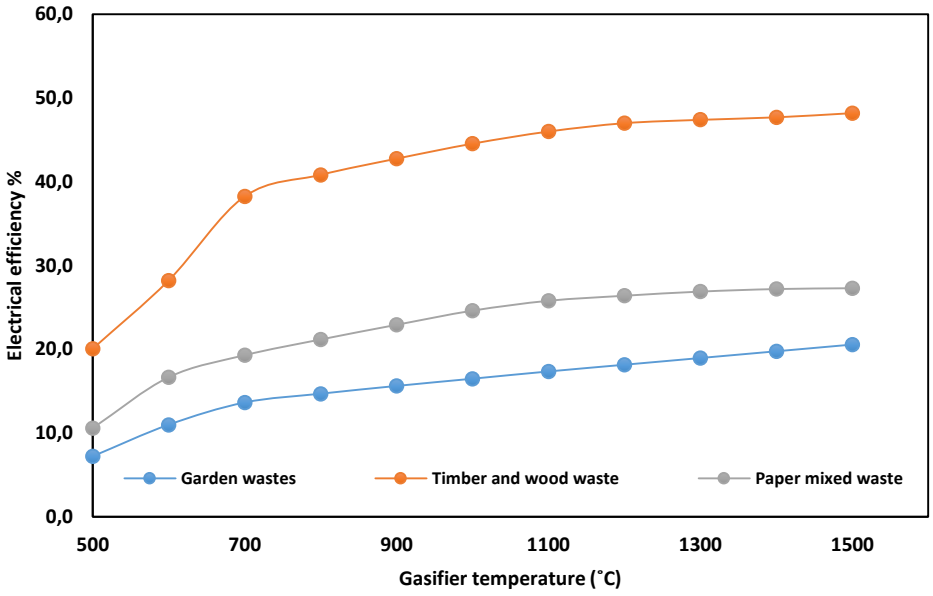


Figure 4-7. Effect of temperature on power efficiency output from the biowaste gasification (1 ton input of feedstock and 2.5 air to biomass ratio)

At the next step, the effect of air equivalence ratio (ER) on power efficiency of the system is evaluated. As it explained in Section 4.1.2.2, H_2 and CO flow rates decrease with an increase in ER, while CO_2 and CH_4 flow rates increase with an increase in ER. Increased oxygen supply enhances carbon and hydrogen oxidation reaction. These two reactions utilize carbon and hydrogen to produce CO_2 and H_2O; then the syngas production and consequently power generation decline. Hence, it is important to find the appropriate range of ER for biomass gasification. In this case, the ER in the gasifier was varied from 0.2-0.65 and its influence on the power efficiency are shown in Figure 4.10 for the three wastes. As shown in Figure 4.10 the optimum ER lies between 0.25-0.3, 0.4-0.5 and 0.35-0.45 for timber and wood, paper mixed and garden wastes, respectively. At optimum span of ER, the power efficiency from gasification of timber and wood waste is higher than that of paper mixed and garden wastes averaging 42% and 63%, respectively.

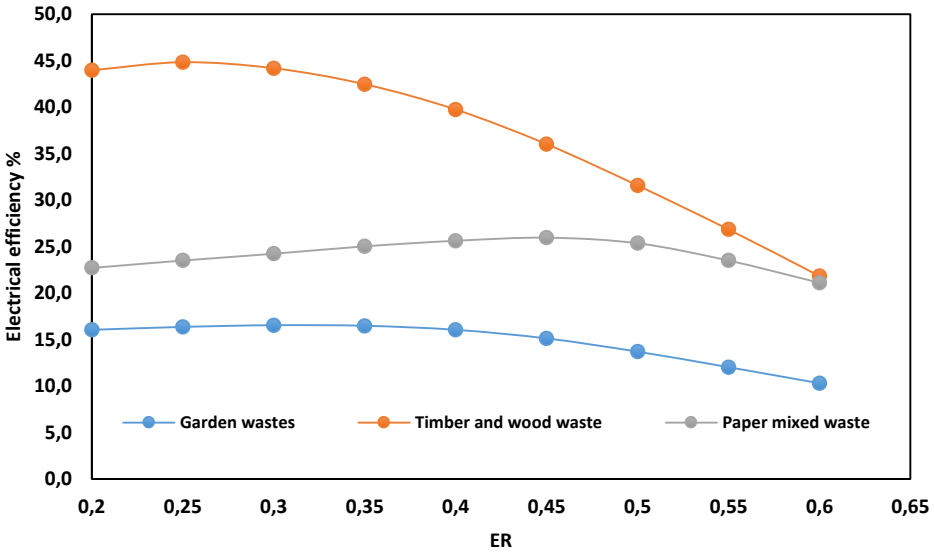


Figure 4-8. Effect of ER on power efficiency output from the biowaste gasification (1 ton input of feedstock and 2.5 air to biomass ratio)

4.3 Environmental assessment

The environmental impact assessment of the integrated gasification with power production unit has been analyzed with the three categories of global warming, acidification and eutrophication potentials. This assessment was directed based on a functional unit of 1 ton of input feedstock and under the optimum operating conditions obtained in Section 4.2.2 for each waste. Discussion in relation to each impact category is presented in the following.

4.3.1 Global warming potential

The GWP comparison of gasification integrated with power unit for the studied wastes with the direct combustion of them and their GWP contributions through the gasifying are shown in Figures 4.11 and 4.12, respectively. Garden waste with GWP of 56 $kgCO_{2eq}$ per ton has the highest GHG emissions. This is due to garden waste having the highest moisture content (50%) and requiring more energy for drying leading to higher GHG emissions releasing to the atmosphere. The largest contribution for all wastes is made by transport through consumption of diesel fuel following with cutting, handling and drying in preparation process. Of the process chain, conversion 2 including the combustion chamber, gas and steam turbines makes up the smallest share of GWP contributions because when biomass is burnt, carbon dioxide releases back to the atmosphere but this biogenic CO_2 is not counted as a contributor to global warming. As seen in Figure 4.11, on a per ton of raw feedstock basis, the degree of reduction in global warming if gasification is used instead of direct combustion is around 90%. Obviously, the production of electricity from waste based on gasification technology appears to be more environmentally friendly than waste direct

combustion if GWP is evaluated. This is because gasification technology has a lower level of exhaust emissions of significant air pollutants and a higher amount of carbon retained in the ash.

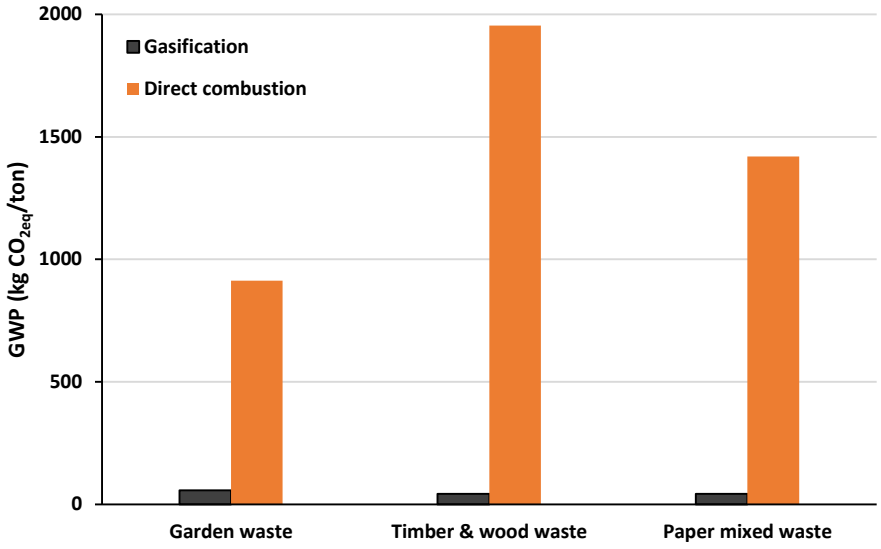


Figure 4-9. GWP of waste gasification for electricity production versus waste direct combustion

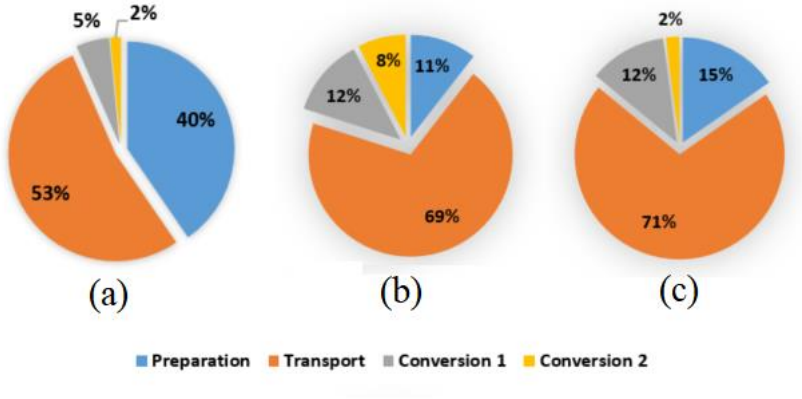


Figure 4-10. GWP contributions for 3 wastes gasification: (a), garden (b), timber & wood (c), paper mixed

4.3.2 Acidification potential

The comparison of electricity production from waste relying on gasification versus direct combustion in relation to acidification potential impact is presented in Figure 4.13. Regarding this index, the production of electricity from garden, timber and paper wastes gasification create 16, 54 and 12 $kgSO_{2eq}$ per ton of raw feedstock, respectively. The emissions of acidic gases from the combustion process in the conversion 2 sector accounts for a major share of the impact, leaving a relatively minor share to the other processes. As

seen in Figure 4.13, CHP gasification of timber and wood waste has the worst AP impact. This is because the highest amount of acidic gasses like NO, NO_2, SO_2 and HCL are released to the atmosphere. However, it is still much more environmentally friendly in comparison to direct combustion.

Figure 4-11. AP of waste gasification for electricity production versus waste direct combustion

4.3.3 Eutrophication potential

In Figure 4.14, the eutrophication impact is compared for CHP gasification of three different wastes versus wastes combusted directly. Production of electricity from consumption of 1 ton of garden, timber and wood wastes in gasification releases 98, 225 and 141 $kgNO_{3eq}$, respectively. The most important contribution to this impact is made by the emissions of particulate matters, N_2, NO_3, NO and NH_3 from the combustion process, whereas the contribution made by the other processes, preparation, transport and gasification is relatively minor.

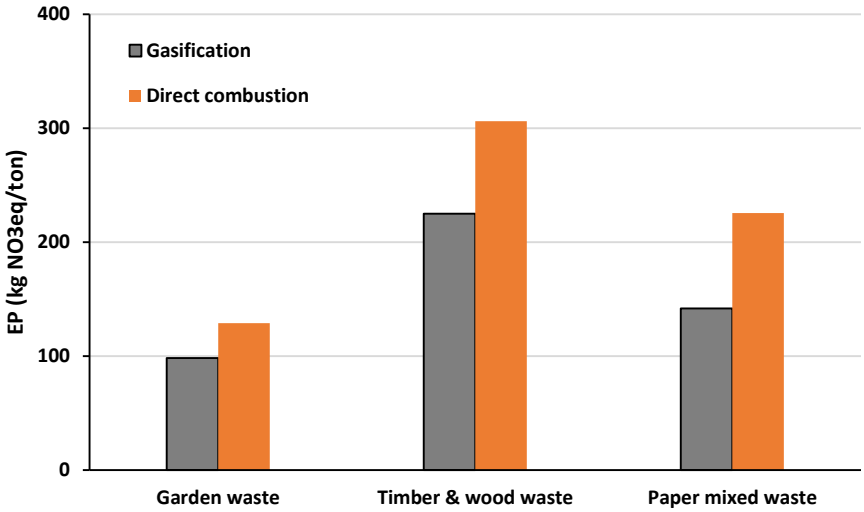


Figure 4-12. EP of waste gasification for electricity production versus waste direct combustion

To have a more accurate comparison of different feedstocks, the environmental impacts per kWh electricity produced in the three studied waste-gasification process is displayed in Figure 4.15. As seen in Figs. 21, 22 and 27, timber and wood waste is the most beneficial from the performance and environmental perspectives. At various temperatures and equivalence ratios, the system based on timber and wood waste has the highest statues in electrical efficiency, as well as lowest levels of in pollutant gas emissions among the other systems. This can be explained by the fact that this kind of waste contains high level of carbon and hydrogen which leads to high power production and also includes a fair amount of moisture which causes it to require lower energy for drying in the preparation sector leading to slight GHG emissions releasing to the atmosphere.

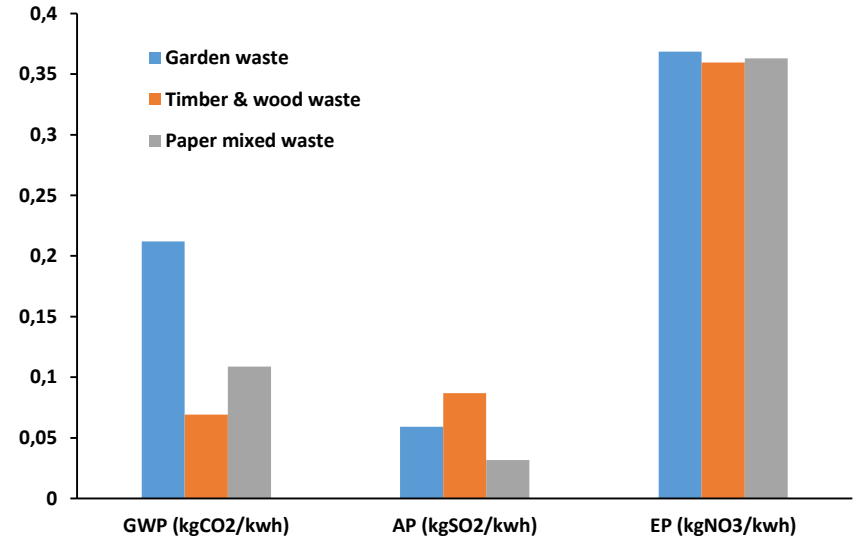


Figure 4-13. GWP, AP and EP of waste gasification per 1 kWh net power production

4.4 Techno-economic assessment

4.4.1 Case study

In this part, the techno-economic assessment of timber and wood waste (T&WW) gasification for energy production in small communities in Iceland is carried out. T&WW has been selected for evaluation because as it has been shown in Section 4.3, this kind of waste is the most beneficial from the performance and availability perspectives among the different gasification systems based on various wastes in Iceland.

Timber waste is generally defined as unpainted and painted timber and is produced from construction/demolition work, packaging waste and pallets. The total amount of timber waste in Iceland in 2010 has been estimated to around 37 ± 11 thousand ton and it has been projected to reach approximately 49 ± 15 thousand ton in 2030. Wood waste is also available from forestry, and it has been estimated to nearly 8,260 ton/year. Totally, timber and wood waste mainly consist of softwood, with a composition of 45% cellulose, 22% hemicellulose and 28% lignin as well as extractives, acids, salts and minerals. Hence, all produced T&WW can be considered as potential for syngas production [1].

There are 72 municipalities in Iceland that their population varies from 43 inhabitants in the smallest ones, to more than 126,000 in the biggest. About 55% of Icelandic municipalities have lower than 1,000 residents and 70% of them occupies lower than 2,000 populations. In these kinds of regions where wide grid is not feasible, small-scale gasification integrated with power generation offers a viable option for meeting the electricity needs of the local population [5].

In order to have a wide evaluation of the economic feasibility of the installation of gasification facilities for all disparate Icelandic zones, 35 subgroups based on various number of households/inhabitants (Table 4.3) were established. In each subgroup, the study was conducted over hypothetical cases, according to the number of households as each household includes 5 persons.

4.4.2 Technical performance

The calculations performed in this paper show that it is beneficial technically and energetically to produce electrical power from the waste biomass downdraft gasification integrated with power generation. Whether this technology can be successfully applied for the purpose of electricity distribution in small municipalities geographically isolated depends on economic and environmental considerations.

The yearly electricity consumption per capita in the household sector in Iceland is around 2.5 MWh per capita. Based on this data, Iceland occupies the forth place in electricity consumption in the world (Norway, Sweden and Finland have the first, second and third statues, respectively) [160]. By using this data, the yearly electricity consumption and power

demand for each subgroup was calculated and shown in Figure 4.16. Obviously, as the population grows, energy demand also increases. Power demand varies form 14,3 kW for the first subgroup with 50 persons (10 households) to 499,4 kW for the last one with 1750 persons (350 households).

Table 4-3. The considered subgroups with the number of household and population

Subgroups	household	persons	Subgroups	household	persons
1	10	50	19	190	950
2	20	100	20	200	1000
3	30	150	21	210	1050
4	40	200	22	220	1100
5	50	250	23	230	1150
6	60	300	24	240	1200
7	70	350	25	250	1250
8	80	400	26	260	1300
9	90	450	27	270	1350
10	100	500	28	280	1400
11	110	550	29	290	1450
12	120	600	30	300	1500
13	130	650	31	310	1550
14	140	700	32	320	1600
15	150	750	33	330	1650
16	160	800	34	340	1700
17	170	850	35	350	1750
18	180	900			

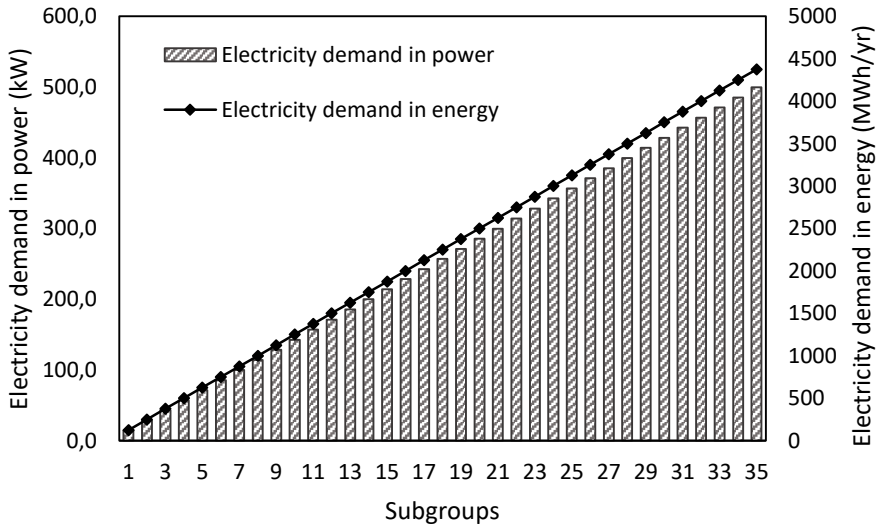


Figure 4-14. Electrical energy and power demand for each subgroup

By considering the demanded power for each subgroup and existing gasifiers capacities (Section 3.4), the required gasifiers capacities which need to be installed for each case have been extracted and depicted in Figure 4.17. As a constraint, more than two gasifiers have not been taking in account for each subgroup. For example, one gasifier with 20 kW capacity has been selected to satisfy 14,3 kW as the requested power for the first subgroup. However, for the second subgroup, two gasifiers with 5 and 25 kW need to be installed to supply 28,5 kW demanded. Analyzing the subgroups 9 and 10 shows that, it is possible that both have the same installed power (150 kW), equally two gasifiers with 100 and 50 kW were considered for both with the requested power of 128,4 and 142,7 kW, respectively. The same happens for the cases of 6 and 7 (100 kW), 11 to 14 (200 kW), 16 and 17 (250 kW), 18 to 21 (300 kW), 22 to 24 (350 kW), 25 to 28 (400 kW), 29 to 31 (450 kW) and 32 to 35 (500 kW).

Figure 4.17 also shows the relation between the installed power and the amount of T&WW that is fed to the system for treatment and power production. Clearly, the installed power does not increase in the same proportion that the input waste, due to different capacity used for each system. For some cases, the installed gasification capacities are oversized, so the required investments of the capital costs and O&M costs need to be considered dependent upon the components size.

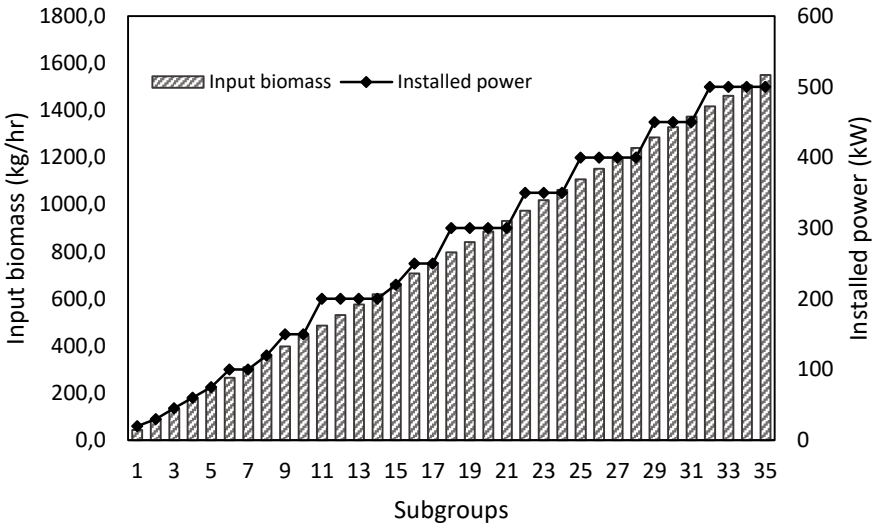


Figure 4-15. Input T&WW and installed power for subgroups

4.4.3 Economic assessment

4.4.3.1 Costs and revenues

The total cost of the generation plant for each population subgroup for the basic scenario (scenario 1), is shown together with the corresponding installed power in Figure 4.18. The total cost varies from about 1100 k€ (Subgroup 1) to more than 2000 k€ (Subgroup 35). The total cost increases as the installed power grows, this trend is kept till up 5, but subgroups 6

and 7 present relatively lower cost in comparison to the former subgroup. It can be explained that the requested power of these subgroups (100 kW) are met only by using one gasifier. This is also similar for the subgroups of 11-14 (200 kW), 18-21 (300 kW), 25-28 (400 kW), and 32-35 (500 kW).

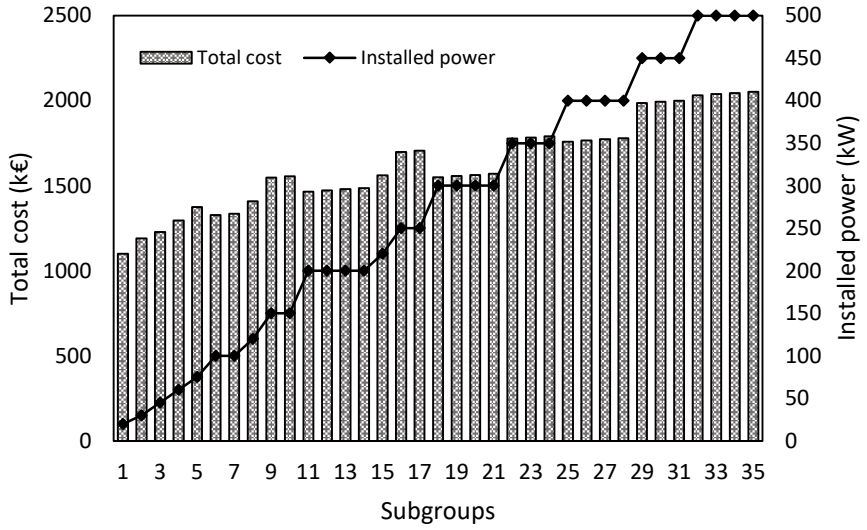


Figure 4-16. Total costs on the basis of the installed power for scenario 1

Percentage shares depicted in Figure 4.19 are contributions of hardware, installation, engineering and annual O&M costs in total cost for basic scenario. The yearly O&M costs occupies more than 70% of total cost for the first subgroup, it has also the dominant statue among different kinds of costs for subgroups 1-8. However, the highest share is related to gasification system price for subgroups 9-35.

Figure 4.20 presents the specific cost for the implantation of new facilities for power production by using T&WW gasification, per ton of waste treated. It has been pointed out that the specific cost per ton of T&WW is inversely proportional to the installed capacity, at higher installed capacity lower the specific costs. Figure 4.20 also shows the specific costs per capita, indicating that for lower population, higher cost per inhabitant is required.

If decision makers want to implement the gasification technology in Icelandic cities, a viable solution for the subgroups 1-5 to reduce the specific costs could be to make connection between neighbour municipalities by making commons investments for bigger gasification facilities, where the T&WW of two or three municipalities could be gasified together.

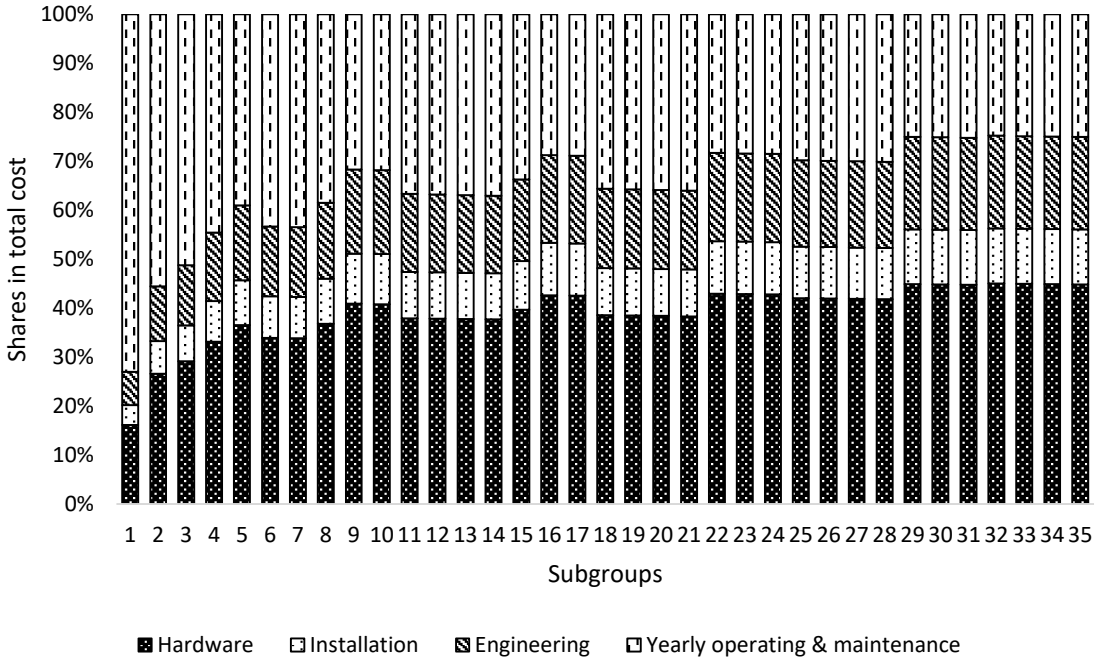


Figure 4-17. Percentage shares of total cost for scenario 1

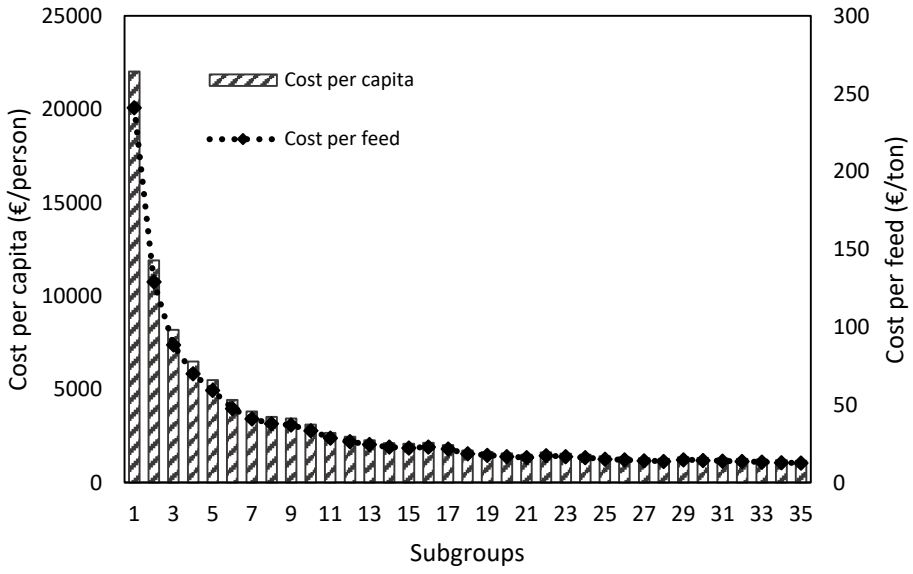


Figure 4-18. Specific cost of T&WW gasification per input waste and per capita

Regarding to revenues, they are obtained by commercialization the generated electricity through the T&WW gasification and the WTB fee for the treatment and disposal of T&WW. Table 4.4 shows the revenues of the sale of electricity, the WTB fee and total revenue for each subgroup. The revenues have a direct relation with the amount of T&WW production and treated per year, since the higher the input waste, the higher the products. The amount

of treated T&WW varies from 304.5 ton/year (subgroup 1) to 10,851.5 ton/year (subgroup 35).

Selling of electricity varies from 12.5 k€ (subgroup 1) to 437.5 k€ (subgroup 35) and the gains because of WTB fees for the T&WW treatment, range from 39.6 k€ (subgroup 1) to 1,410.7 k€ (subgroup 35). It is worth mention that for all subgroups the incomes obtained with the WTB fee is equivalent to more than 70% of total revenues.

Table 4-4. The annual revenue based on sale of electricity and waste treated

Subgroup	Income with sale of electricity (k€/year)	Income with WTB (k€/year)	Total income (k€/year)	Subgroup	Income with sale of electricity (k€/year)	Income with WTB (k€/year)	Total income (k€/year)
1	12,50	39,59	52,09	19	237,50	765,47	1002,97
2	25,00	79,91	104,91	20	250,00	805,79	1055,79
3	37,50	120,24	157,74	21	262,50	846,12	1108,62
4	50,00	160,57	210,57	22	275,00	886,44	1161,44
5	62,50	200,89	263,39	23	287,50	926,77	1214,27
6	75,00	241,22	316,22	24	300,00	967,10	1267,10
7	87,50	281,55	369,05	25	312,50	1007,42	1319,92
8	100,00	321,87	421,87	26	325,00	1047,75	1372,75
9	112,50	362,20	474,70	27	337,50	1088,08	1425,58
10	125,00	402,53	527,53	28	350,00	1128,40	1478,40
11	137,50	442,85	580,35	29	362,50	1168,73	1531,23
12	150,00	483,18	633,18	30	375,00	1209,06	1584,06
13	162,50	523,51	686,01	31	387,50	1249,38	1636,88
14	175,00	563,83	738,83	32	400,00	1289,71	1689,71
15	187,50	604,16	791,66	33	412,50	1330,04	1742,54
16	200,00	644,49	844,49	34	425,00	1370,36	1795,36
17	212,50	684,81	897,31	35	437,50	1410,69	1848,19
18	225,00	725,14	950,14				

4.4.3.2 Economic assessment of three scenarios

To have a comparison between different scenarios, the total cost required for power generation based on T&WW gasification, during the period of analysis, for each subgroup are shown together in Figure 4.21. Higher interest rates tend to reduce total cost during 15 years of operation. The total costs, with the interest rate of 8% for Scenario 1 range of 1100 k€ (subgroup 1) to 2050 k€ (subgroup 35), the costs with interest rate of 10% for Scenario 2 range of 983 k€ (subgroup 1) to 1882 k€ (subgroup 35), and total costs with interest rate of 13% for Scenario 3 range of 842 k€ (subgroup 1) to 1680 k€ (subgroup 35). In fact, for the higher interest rate, the smaller present investment is required to achieve the revenue required for the project to succeed. However, the costs alone do not reflect economic-

effectiveness of the project. The costs, revenues and their effects together on NPV need to be investigated to demonstrate which project is the most beneficial from the economic perspectives.

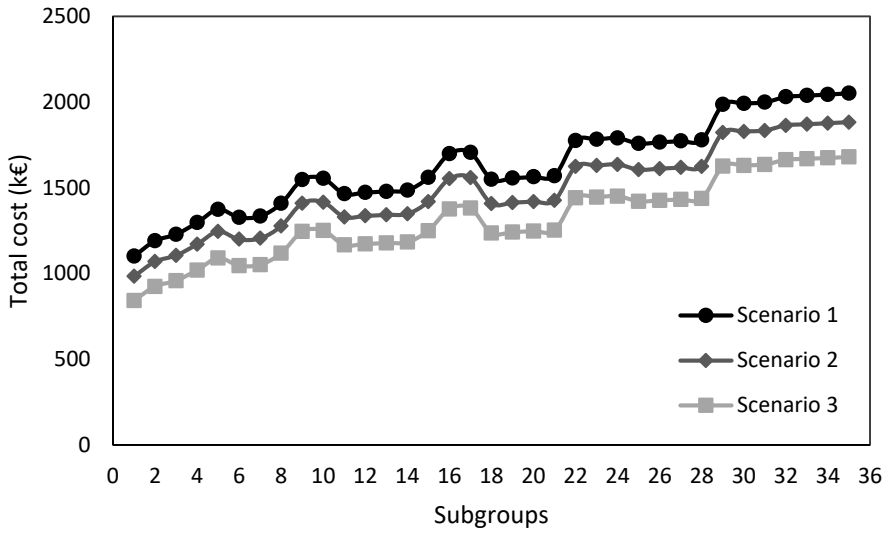


Figure 4-19. Total cost required for power generation based on T&WW gasification for different scenarios based on different interest rates: 8% in Scenario 1, 10% in Scenario 2 and 13% in Scenario 3

The economic assessments, based on the indexes of NPV and DPP for scenarios 1, 2 and 3, are shown in Figures 4.22, 4.23 and 4.24, respectively. Different from the discount rate, NPVs for three scenarios are positive in 94% of the subgroups (3–35) and negative in the remaining 6% (1 and 2). In the other words, implementation of T&WW gasification integrated with power generation unit in Iceland could be economic beneficial projects for places with more than 150 inhabitants or for installed capacities higher than 45 kW. It is worth noting that, in scenario 1 with the interest rate of 8%, NPV is averagely 11% and 25% greater than scenarios 2 and 3, respectively.

In addition, changing the interest rate does not have significant impact on DPP for all studied scenarios; it is lower than 2 years in 88% of the subgroups (5–35) and attractively it is lower than 6 months from subgroup 13 reducing to 4 months for subgroup 35. These all show that employing small scale T&WW gasification could be an economic alternative in Icelandic municipalities.

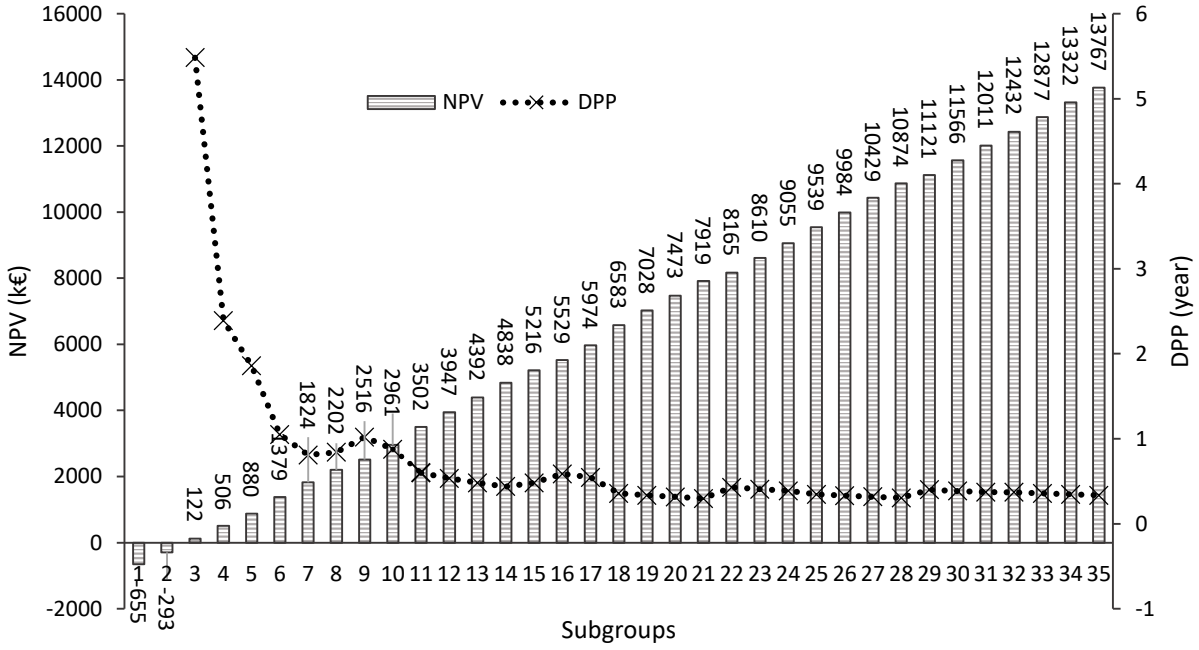


Figure 4-20. Economic analysis for scenario 1 with interest rate of 8%

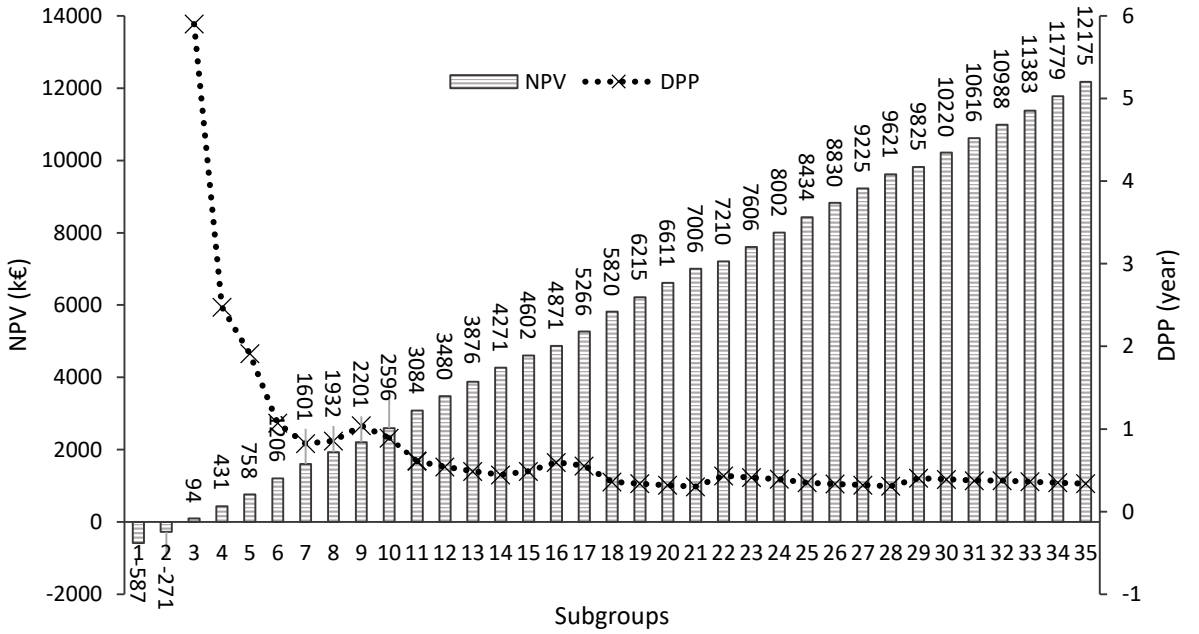


Figure 4-21. Economic analysis for scenario 2 with interest rate of 10%

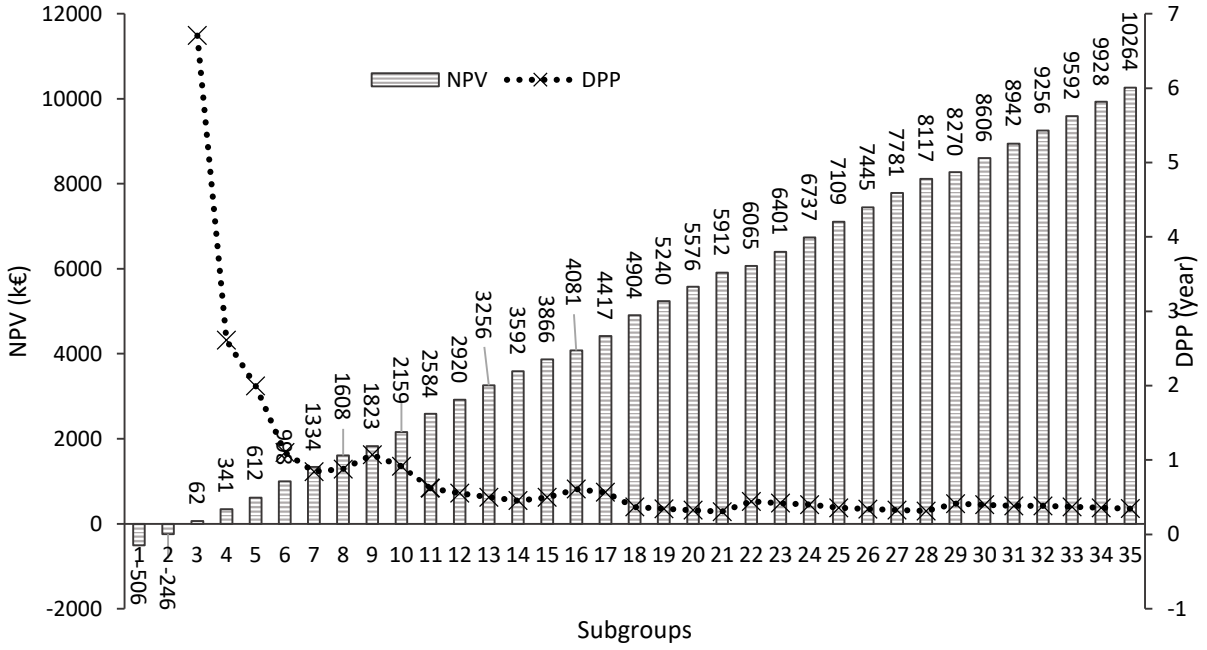


Figure 4-22. Economic analysis for scenario 3 with interest rate of 13%

The subgroups that do not show economic feasibility for these scenarios, could have the strategy of merging in municipalities to reduce the costs and increasing the yields, then looking after the possibility of a higher amount of waste and making viable to install a treatment facility. Another way is to establish a minimum value for the fee of waste collection and disposing. Hence, it was carried out a sensitivity analysis, to find the minimum WTB, to have viable installation of a hypothetical T&WW gasification plant, independent of its size (Table 4.5). The minimum WTB varies from about 380 € per ton of waste (subgroup 1) for all scenarios to zero from subgroup 14 in scenario 1, subgroup 15 in scenario 2 and subgroup 17 in scenario 3. In the other words, in places with more than 700 inhabitants or with the higher installed capacity of 200 kW, projects could be run economically without receiving any fee for collection and disposal of waste.

Table 4-5. Minimum WTB for treatment of T&WW to get a NPV more than zero

	Minimum WTB (k€/ton)		
Subgroup	**Scenario 1**	**Scenario 2**	**Scenario 3**
1	0,381	0,384	0,387
2	0,186	0,188	0,192
3	0,115	0,117	0,120
4	0,082	0,084	0,087
5	0,063	0,065	0,069
6	0,043	0,045	0,047
7	0,032	0,033	0,035
8	0,026	0,027	0,029
9	0,025	0,026	0,029
10	0,018	0,020	0,022
11	0,010	0,011	0,013
12	0,006	0,007	0,008
13	0,003	0,003	0,005
14	**from 14-35 is zero**	0,001	0,002
15		**from 15-35 is zero**	0,001
16			0,003
17			**from 17-35 is zero**

5 Conclusions

In this project the problem of a sustainable solution for waste disposal in Iceland was addressed. The process considered is sustainable green gasification technology which is a waste-to-energy system that not only involves wastes as fuel but also helps results in a net reduction of released pollutants. Gasification's potential has been studied in medium-scale facilities by several researchers but only a few successful small-scale studies exist in the literature and also before this project no research has been directed on environmental and techno-economic assessment of small-scale gasification. Hence, the challenges for local waste gasification are its adaption to the Icelandic scale, feedstock and operational parameters. Downscaling must be done while still eliminating the pollution problems of incinerators and the cost constraints of small-scale plants. The key to develop this technology is to overcome the problems associated with technical and economic aspects of power production especially for small-scale plants as well as environmental acceptance.

The global academic value of this project is that it brings the detailed knowledge about the simulation modeling of the small-scale gasification, its performance under various conditions and its environmental and techno-economic assessment, to the world where there is after all many other smaller communities with similar waste streams and waste disposal challenges. In Iceland the results of this study can be used by SORPA or other waste-disposal companies outside Reykjavik, including smaller places such as Vestmannaeyjar and Vestfirðir. It provides a green solution for disposing of significant amounts of waste and for mixing diverse feedstocks, including painted and treated wood (about 40.000 tons per year), without the methane emissions and groundwater leaching of landfilling or the air pollution and toxic residues of incineration. It could lead to a sustainable waste-management system that preserves a relatively pristine environment in Iceland. Moreover, before this project no research has been done on environmental and techno-economic assessment of small-scale biowaste gasification as well as its integration with power production unit. Beneficially, this project has a practical value that prove the production of electricity from biowaste gasification linked with power unit could be a feasible, environmentally and economic acceptable option to be implemented instead of incinerators and landfilling sites for waste disposal in Iceland. Small scale gasification can meaningfully contribute to energy supply in low populated regions in the world that are far from the central energy networks and need to have a district heat and power system.

Therefore, in this work by using ASPEN Plus simulator, a simulation model was developed for waste biomass gasification integrated with power production unit as an attractive method for high efficiency electricity generation in low populated areas. The model was applied for optimization of the gasifier performance, evaluation of effect of operating parameters and different feedstocks on the syngas composition, the system performance and the overall electrical efficiency. Finally, to propose a sustainable waste to power system adapted with conditions in Iceland, a comprehensive assessment of environmental and economic feasibility of these systems were carried out.

5.1 Answers to the research questions

When going back to the original research questions, one can see that they have been answered in various sections. In this part, the research questions and their brief responses based on their contributions in the papers are brought cohesively as following:

RQ1: What are the waste feedstocks that can be fed to the gasifier?

One part of Paper I, a potential evaluation of organic wastes which are produced in Iceland and can be used for biofuel production, tackles the first research question. This part was also presented in Section 3.2.2 Case study. Organic waste from households, industry and services is a valuable source for biofuels production in Iceland. The Icelandic Environmental Agency set up a national plan to reduce the amount of organic wastes that are landfilled or incinerated over the years. A general estimation shows that approximately 60% of the total waste is organic material of which 70% is obtained from industry and services and 30% is from the household sector. Categories of organic waste from household, industry and services are defined as, garden waste, timber and wood waste, mixed paper waste, fish waste, meat and slaughter waste, kitchen waste, and waste bio oil. Among these organic wastes, garden waste, timber and wood waste, and mixed paper waste are the main wastes that can be fed to a gasifier. Moreover, the total amount of paper, timber and garden wastes in Iceland in 2015 have been calculated as approximately 37, 40 and 16 thousand tons, respectively, and they have been estimated to increase to about 47, 49 and 20 thousand tons by 2030 assuming 0.8%, 0.6% and 0.6% growth rate per capita, respectively.

RQ2: What is the best modelling approach?

Papers II and III investigate on the response of RQ2. Various approaches for biowaste gasification modelling were studied in Paper II to determine which are appropriate based on the type of gasifier, feedstock, operational parameters and tar formation. Moreover, tar modelling in gasification models was studied in Paper II and classified in different ways in a given application. A detailed methodology characterization that includes consequential modelling choices was also introduced and stoichiometric and nonstoichiometric models lead to identical predictions or not were addressed in Paper III. Complete details about the responses of RQ2 has been brought in Section 2.2 Biomass gasification models. Briefly speaking, the equilibrium modelling method has been used to predict reliably downdraft fixed-bed gasifier performance as a function of feedstock and given information about operational conditions.

RQ3: What are the optimal settings of operating parameters on the gasification technology?

Papers of IV and V study on the responses of the RQ3. This part was also presented in Section 4.1 Primary model. In these papers a primary simulation model for biowaste gasification has been developed to predict the system performance, fluid flow, heat transfer and process patterns and to evaluate the effects of various operating conditions such as

temperature, equivalence ratio, moisture content and waste composition influence on the produced gas composition, overall system efficiency and system performance. In summary, raise in temperature improves the gasifier performance, it increases the production of CO and H_2 which leads to higher syngas yield, LHV and CGE. However, Increasing ER lessens the production of CO and H_2 which results in reduction of gasification performance. The optimal values of CO and H_2 mole fraction and CGE of several feedstocks like sawdust, wood chips and mixed paper wastes are located at 900, 1000 and 1000 ˚C, respectively and ER range is between 0.20-0.35 regardless of the kind of biomass which is used as the feed-stock. Among the studied wastes, while wood chips waste has the highest carbon percent among the other wastes, it has slight carbon yield, low CO mole fraction as well as lowest LHV. It is due to it includes so high amount of moisture and moisture content indirectly effects on LHV of syngas, increasing moisture content strongly degrades the syngas LHV. Moreover, mixed paper waste shows the highest CGE (70.6%) at temperature of 1000 ˚C because of much higher hydrogen content and less HHV of its feedstock while wood chips show lowest CGE, around 60%.

RQ4: What are the effects of several inputs on the power output from the system?

To tackle the RQ4, an upgraded simulation model was developed for integrated biowaste gasification with power production unit to assess performance of producing electricity from gasifying of various types of organic wastes in Iceland. The objectives are finding the optimal operating conditions (type of feedstock, gasifier temperature, equivalence ratio and moisture content in biomass) to make highest electrical efficiency. The results of these part have been published in papers of VI, VII and X and also presented in Section 4.2 Advanced model. Simulation results indicate that optimal operating conditions for producing the highest power efficiency are gasifier temperatures of 900-1000 ˚C for the studied wastes and an equivalence ratio between 0.2-0.3, 0.4-0.5 and 0.35-0.45 for timber and wood, paper mixed and garden wastes, respectively. At the optimum range of temperature and ER, the power efficiency from gasification is 45, 26 and 16% for timber and wood, paper mixed and garden wastes, respectively.

RQ5: Is small-scale gasification an environmentally sound solution?

In order to solve the RQ5, an environmental assessment of energy recovery through the biowaste gasification integrated with power production unit was carried out and results reveal that the considered appears to be more environmentally friendly than waste incineration in all impact categories considered. This can be explained by the fact that gasification technology has a lower level of exhaust emissions of significant air pollutants and a higher amount of carbon retained in the ash. Among the systems, timber and wood waste is the most beneficial from the performance and environmental perspectives. The production of 1 kWh of electricity from timber through gasification would lead to a GWP of 0.07 kg CO_2eq, AP of 0.09 kg SO_2eq, and EP potential of 0.36 kg NO_3eq. Of the processes in the chain, the largest contribution for all wastes is made by transport through consumption of diesel fuel following by cutting, handling and drying in the preparation process. Whereas

the second conversion containing the combustion chamber, gas turbine occupies the smallest share in environmental contributions. Results of environmental assessments (response to RQ5) were published in paper VI and also discussed in Section 4.3 Environmental assessment.

RQ6: Can small-scale gasification be made techno-economically feasible?

To answer the RQ6, a comprehensive assessment of techno-economic feasibility adapted with conditions in Iceland for the gasification facilities integrated with electricity generation unit was directed. The technical assessment focused mainly on input waste, installed power, and electrical power generation. The economic assessment was conducted relied on the economic indicators of total cost, specific costs, revenues, net present value (NPV) and discounted payback period (DPP), bringing together different economic scenarios, with different interest rates. Additionally, a sensitivity analysis was carried out, to investigate the effects of the fee paid by the Icelandic municipalities for collection and disposal of wastes (WTB).

The results of techno-economic assessment show that changing the interest rate does not have significant impact on NPV and DPP for all studied scenarios. the NPV is positive for a gasification system with the capability to generate greater than 45 kW. The NPV in scenario 1 (8% for interest rate), is averagely 11% and 25% higher than scenarios 2 and 3, respectively. Discounted payback period (DPP) will be also lower than 2 years for a gasification with capacity higher than 75 kW. However, it could be lower than 6 months if gasification is applied in capacity greater than 200 kW. The results from techno-economic analysis (response to RQ6) were brought in papers VIII and IX and also discussed in Section 4.4 Techno-economic assessment

5.2 Future work

A highly desirable next step is that the simulation model developed in this work is validated by the experimental data which will be generated at the biowaste pilot gasifier recently commissioned at the University of Iceland. Currently, this pilot-scale gasifier is the only operational gasifier in Iceland. The gasifier and CHP system has been commissioned early 2020 and currently the gas composition and tar sampling systems are being installed and calibrated. In fact, validation of the model with the experimental data obtained from this UI gasifier would identify model strengths and failures and confirm how accurate and reliable the predictions of each step in the model developed here is. Refinement based on experimental input could lead to a model that is sufficiently complete and correct to support the system development and optimization.

Additional recommended future work is the introduction of downstream technology to further process the syngas and for example produce value added products like biofuels. Syngas purification and conversion technologies help enable biofuel extraction and

increased value from the energy in waste and contribution to a sustainable energy supply. With these addition gasification systems could produce different biofuels such as biohydrogen, biomethane, bioethanol and biodiesel. Biomethane could be purified after passing of syngas from the methane recovery/capturing plant. Similarly, in another alternative, hydrogen could be purified after passing of syngas from the H_2 recovery/capturing unit. Moreover, biowastes can be converted into bioethanol by passing of syngas from syngas fermentation and product recovery units. Biodiesel can be also produced through the integrated gasification and the Fischer-Tropsch process.

At the next step, a simulation tool needs to be used to model all the alternative systems to evaluate the effects of several feedstocks and operational parameters on maximum output. Development of a simulation model as a main step speeds up the process of finding optimal conditions, as it is impractical to test every condition and material in experiments. Then, a sustainability assessment of energy recovery from the waste through the different alternative systems need to be carried out to rank different system based on different sustainability perspectives and to propose a sustainable waste to energy system adapted with conditions in Iceland.

5.3 Thesis limitations

It is important to mention that the simulation model developed in this work models downdraft gasification and it cannot be employed for other types of gasifiers like fluidized bed and updraft gasifiers. Because the objective of this project was using gasification in at small-scale/low capacity, downdraft gasification was selected that since it is currently the most widely gasifier type used on small scale and arguably the most economical and suitable among all gasifier types for small-scale operations. Hence, if the gasification used for waste disposal is in medium or large scale, it is required to also consider fluidized bed gasification. A sufficiently reliable model of fluidized bed gasification to be practically useful likely would have to simulate both fluid-dynamic and reaction kinetics simultaneously. In fact, a drawback of using equilibrium modelling utilized for downdraft gasifier is its inability to evaluate the hydrodynamic parameters of biomass gasification, so a prediction of hydrodynamic phenomena in the fluidized bed gasifier (moving to a kinetic approach) would be helpful. For this kind of gasifier, a kinetic model needs to be developed to learn more about the effects of particle size, density, carbon conversion, electricity production and the reactivity of the syngas.

Moreover, in this project the integration of just electrical power production with gasification has been considered. However, if cogeneration of heat and power (CHP) is linked to the main system, the discounted payback period (DPP) could be much lower (in locations where heat or hot water have a premium, too) and gasification could be even more feasible than shown here due to both power and hot water adding revenue.

Despite the above-described limitations, this study has proposed a sustainable waste-management system that preserves a relatively pristine environment in small communities like Iceland. Moreover, before this project no research has been done on environmental and techno-economic assessment of small-scale waste biomass gasification as well as its integration with power production unit. Beneficially, this project has a practical value that prove the production of electricity from waste biomass gasification linked with power unit could be a feasible, environmentally and economic acceptable option to be implemented instead of incinerators and landfilling sites for waste disposal. It can be applied for energy supply in low populated regions in the world that are far from the central energy networks and need to have a district heat and power system.

6 Papers

Paper I

An assessment of the sustainability of lignocellulosic bioethanol production from wastes in Iceland.
Safarian, S., & Unnthorsson, R. (2018)
Energies, 11(6), 1493

energies

MDPI

Article

An Assessment of the Sustainability of Lignocellulosic Bioethanol Production from Wastes in Iceland

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Abstract: This paper describes the development of a model to comprehensively assess the sustainability impacts of producing lignocellulosic bioethanol from various types of municipal organic wastes (MOWs) in Iceland: paper and paperboard, timber and wood and garden waste. The tool integrates significant economic, energy, environmental and technical aspects to analyse and rank twelve systems using the most common pretreatment technologies: dilute acid, dilute alkali, hot water and steam explosion. The results show that among the MOWs, paper and paperboard have higher positive rankings under most assessments. Steam explosion is also ranked at the top from the economic, energy and environmental perspectives, followed by the hot water method for paper and timber wastes. Finally, a potential evaluation of total wastes and bioethanol production in Iceland is carried out. The results show that the average production of lignocellulosic bioethanol in 2015 could be 12.5, 11 and 3 thousand tons from paper, timber and garden wastes, respectively, and that production could reach about 15.9, 13.7 and 3.7 thousand tons, respectively, by 2030.

Keywords: bioethanol; sustainability assessment; lignocellulosic wastes; pretreatment

1. Introduction

Negative social, political and environmental impacts of fossil fuels as well as energy security concerns have spurred interest in nonpetroleum energy sources [1]. Among the various alternative energy sources, biomass has garnered substantial interest because it is the only suitable and renewable primary energy resource that can provide alternative transportation fuels [2]. Bioethanol has long been put forward as the most promising biofuel used either as a sole fuel in cars with dedicated engines or as an additive in fuel blends, requiring no engine modifications until the mix reaches 30% [3].

The main feedstocks of bioethanol are sugar- and starch-based materials such as sugarcane and grains. However, there are considerable debates about the sustainability of such feedstocks. Lignocellulosic materials, a third group of feedstocks, represents the most viable option for bioethanol production. Increasing food demand and the need to feed an increasing global population could make conventional agricultural crops less competitive and more costly sources compared to lignocellulosic materials [4–6].

In this context, municipal organic wastes (MOWs) represent one of the most abundant lignocellulosic materials and acquires significant importance for bioethanol production. The replacement of biomass with MOW can provide environmental advantages, particularly with regard to waste management, carbon dioxide, quality and quantity control of water, land use and biodiversity [7]. However, the as yet immature technologies and challenging logistics for sourcing waste pose barriers to utilizing this potential source [4].

Based on these concepts, this paper focusses on bioethanol production from MOWs in Iceland. Iceland possesses no fossil energy resources, but in comparison to its population of 332,529, the country has huge amounts of hydroenergy and geothermal energy. Economic estimations of the country's hydroelectric energy show that about 30 TWh/year may be harnessed, but only 15% is being used. Likewise, geothermal energy has been estimated at about 200 TWh/year, of which only 1% has been harnessed. Approximately 90% of buildings in Iceland are heated with geothermal water, and the aluminum and ferrosilicon industries are powered by hydroelectric energy, consuming 4.25 TWh/year. However, the transportation and fishing sectors are powered totally by imported fossil fuels [8]. Hence, utilization of biofuel can be useful as a sustainable mode for transitioning to green transportation and fishing infrastructure.

An overview of different Icelandic municipalities is shown in Figure 1a, the Capital area (pink), South peninsula (blue), South (yellow), West (purple), East (orange), Northeast (red), Eyjafjörður (turquoise), Northwest (brown) and Westfjords (green), [8]. Although Iceland is large by land mass, more than 60% of the population lives in the capital area and about 80% live in the capital and south regions combined (Figure 1b). However, the capital area occupies only 1% of the total area of Iceland (Figure 1c). This is due to the development of urbanization in this location, poor climate and geographical conditions in other regions and slow and expensive transportation.

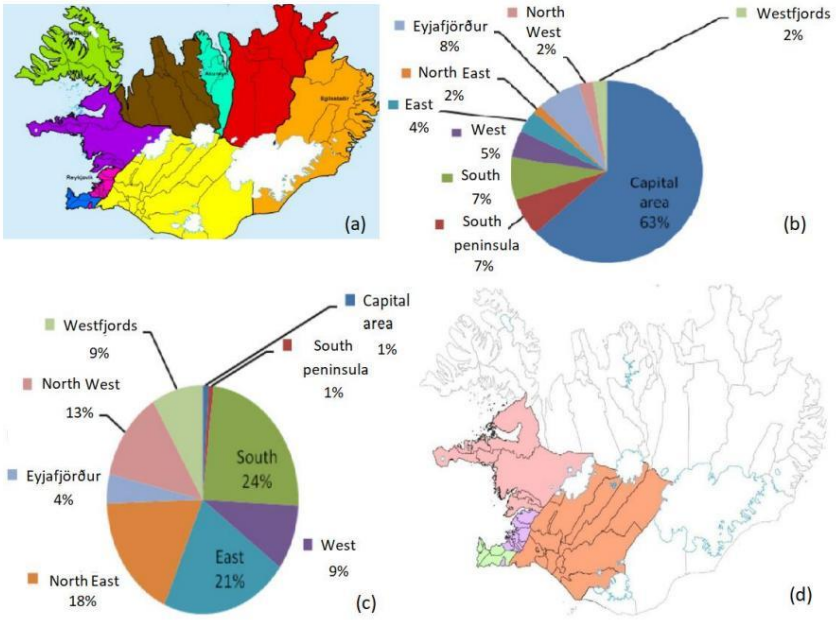

Figure 1. Map and information of Iceland, (**a**) all municipalities, (**b**) population share, (**c**) area share and (**d**) major region.

Climate and weather conditions are more likely to limit farming in Iceland than soil type [9,10]. Even though arable land is available, vast portions of the areas with suitable soil type have climate and weather unsuitable for vegetation growth. In fact, the crop growth window in Iceland is 130 days in the summer (7 May to 15 September). Thus, the only products that can be developed must have a growing time within this period and the temperature required for growth must be compatible with

the environment temperature (5–7 °C). This situation means that grasses turn green and tillage can be performed, but little else is grown [9,11].

Based on these conditions, biofuel production efforts in Iceland should focus on MOW as part of the second-generation biomasses. Despite lack of agricultural crops, waste is recognized as a continual source of biomass and is independent of climate conditions and other immutable factors. Furthermore, because the amounts of various wastes produced in different locations are fairly constant and measurable, reasonable estimation of biofuel production capacity should be possible.

To establish sustainable bioethanol production plans, they should be evaluated from different sustainable development perspectives and compared based on different initial feedstocks and applied conversion technologies. Sustainable production scenarios of bioethanol depend on economic, technical, environmental, social and political factors as well as energy balance and are essential elements of sustainable development [12]. The authors are not aware of any published studies assessing bioethanol production systems based on the sustainable development dimensions in Iceland. Therefore, the goals of this study are: (i) to assess 1-ton bioethanol production using three different Icelandic MOWs: paper and paperboard, timber and wood and garden waste; (ii) to develop a model based on energy and material flows to assess the economic (cost and benefit), energy (energy balance, total input/output energy and energy use efficiency) and environmental (GHG emissions, water consumption and supply rate) sustainability criteria; (iii) to analyse and compare the sustainable impacts of different biomass-derived bioethanol, pretreatments and conversion technologies; and (iv) to evaluate the potential of total waste and bioethanol production in Iceland between 2015 and 2030.

2. System Description

The system considered by the model including all the process steps from resources to end products (see Figure 2).

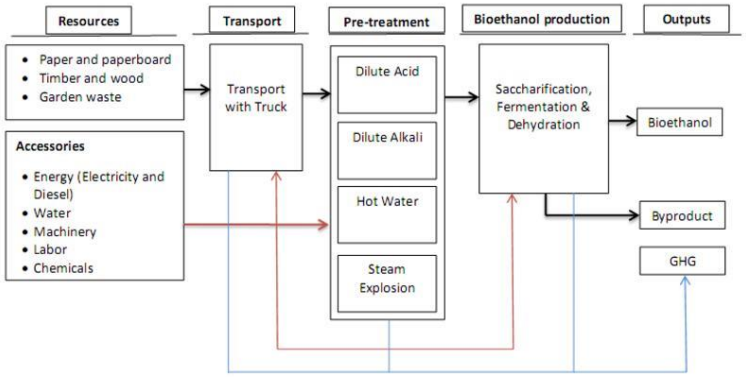

Figure 2. System boundaries considered by in this study including five stages of processes, conversion technologies and associated inputs (energy and material).

2.1. Resource Level

Paper and paperboard, timber and wood and garden waste are considered as the main input resources. According to Icelandic law, all municipalities are obligated to have a waste management plan to organize waste produced in the municipality. Thus, beginning in 2004, common project management groups were established to plan for waste produced in the main municipality parts of Iceland: Western Iceland (pink), Suðurnes (green), the Capital Area (purple) and Southern Iceland

(orange) (Figure 1d) [13]. Waste collection and treatment in these places are mostly operated by four Icelandic companies (Table 1).

Table 1. Information regarding waste operation in the main parts of Iceland in 2006.

Participating Areas	Operator Company	No Municipalities	Waste Quantity (1000 tons)
Western Iceland	Sorpurðun Vesturlands	10	29
Suðurnes	Kalka	5	22
Capital area	Sorpa	8	272
Southern Iceland	Sorpstöð Suðurlands	11	33

About 90% of the wastes generated are related to the capital area and are collected by the Íslenska Gámafélagið and Sorpa companies [14,15]. Due to the low number of inhabitants in Iceland, there is limited economic basis for recycling facilities like paper mills. Plastics and paper items are thus shipped abroad, as there is no facility in Iceland to recycle and reuse them. At present, landfilling and incineration are the dominant methods used for the disposal of municipal solid waste in Iceland, and most landfill sites are open dumping areas, which poses serious environmental and social threats. Moreover, the flue gas from waste incineration can contaminate the environment if not handled with appropriate technologies, such as using combined heat and power (CHP) [16] and flue gas cleaning systems. A small incinerator in Skutulsfjörður at Northwest Iceland resulted in the discovery of cancerous and toxic chemicals in Icelandic meat and milk in 2011 [17]. Dioxin levels in the fly-ash from the nearby incinerator were more than 20 times the EU limits [17]. Moreover, soil and incinerator emissions measurements at several sites in Iceland such as Kirkjubaejarklaustur revealed that emissions were 85 times the EU limits [6,18]. These problematic findings resulted in the widespread testing of soil across Iceland [17], shutdown of several incinerators [18], withdrawal of some Icelandic meat and milk from the markets and culling of all the livestock on the farms impacted [17]. In an attempt to reduce these problems, this study considers diverting paper and paperboard, timber and wood and garden waste as portions of MOW from the waste companies (mostly Sorpa) before they are burnt in incinerators. These materials could then be transferred to preprocessing units and conversion plants to produce bioethanol. Lignocellulosic bioethanol is proposed as a viable alternative to MOWs treatment, and may solve the problems of using huge amounts of land for landfill and high emissions from incineration.

In addition, energy, water, labor, chemicals and machinery are considered accessory inputs. Diesel fuel is used by trucks for transportation and electricity is consumed in driving force and heat generation in process units. It has been reported that 25% and 75% of electricity production in Iceland comes from geothermal and hydropower, respectively. Thus, hydro is currently Iceland's main source of clean energy; however, the electricity required in the capital area, as the largest producer of waste, is supplied by geothermal power plants in Hellisheiði and Nesjavellir [19].

2.2. Transport Level

In this study, the transport step includes waste transport from waste operator companies to preprocessing units. As pretreatment plants and bioethanol production centres should be next to each other, transportation of the liquid containing cellulose from preparation facilities to bioethanol production units is not included.

In this study, a 50 km waste transportation distance by truck is used. The data used for fuel calculations was obtained from published studies [20,21]. The energy equivalent for the transportation of waste is about 3 MJ ton^{-1} km^{-1} (0.06 L ton^{-1} km^{-1}).

2.3. Pretreatment Level

Lignocellulosic materials are composed of cellulose, hemicelluloses and lignin in an intricate structure which is resistant to decomposition. One of the best strategies to convert such biomass

into sugars is enzymatic saccharification due to its low energy requirement and comparatively smaller environmental impact; however, the main problem is the low accessibility of cellulose because of the rigid association of cellulose with lignin [22,23]. Therefore, removal of lignin, making cellulose more accessible to enzymatic hydrolysis for conversion, is the primary pretreatment process investigated herein.

Pretreatment techniques are mainly classified as physical (e.g., grinding and milling), chemical (e.g., alkali, acid, ammonia percolation), physio-chemical (e.g., steam explosion, ammonia fiber expansion) and biological (e.g., fungi and Actinomycetes) [24,25]. Most of these technologies are not preferred for industrial applications due to high energy demand, inability to remove lignin and substantial chemical requirements. Among the pretreatment techniques, dilute acid (DA), dilute alkali (DAL), hot water (HW) and steam explosion (SE) are modeled in this study and are among the most effective and the most promising for industrial applications [23,25,26].

Dilute acid pretreatment is one of the most frequently employed methods of structurally breaking down lignocellulosic biomass and removing the hemicellulose [27]. During this method, biomass is treated at different combinations of temperatures (100–290 °C), at a pressure of 1.5 bar [28], with residence times ranging from a few seconds to several hours. During hydrothermal pretreatment, most of the hemicellulose is hydrolyzed to sugar monomers and becomes soluble, a fraction of cellulose is depolymerized into glucose and a fraction of lignin is dissolved and distributed.

Dilute alkali pretreatment refers to the application of alkaline solutions such as NaOH, $Ca(OH)_2$ or ammonia to remove lignin and a part of the hemicellulose, increasing the accessibility of enzymes to the cellulose. Pretreatment can be performed at low temperatures but with a relatively long residence time and high base concentration [23,24,29].

In the hot water pretreatment method, water under high pressure penetrates the biomass, hydrating the cellulose and removing the hemicellulose and part of the lignin. The method's major benefits are that is does not require chemicals or corrosion-resistant materials for the hydrolysis reactors. Moreover, feedstock size reduction is a highly energy demanding operation for the huge bulk of materials, while there is no need for size reduction in HW pretreatment [23,30].

Among the physico-chemical processes, steam explosion has received considerable attention as a pretreatment for ethanol production. In steam explosion, the pressure is suddenly reduced, causing the materials to undergo explosive decompression. High pressure and high temperature (160–260 °C) are used in steam explosion for a few seconds to several minutes [23,31]. The process has been used in lab and pilot-scale units by several research groups. Moreover, steam explosion has been found effective on feedstock with large particle sizes, thus reducing the energy required for size reduction, and it can satisfy all the requirements of the pretreatment process [24].

2.4. Bioethanol Production Level

After the pretreatment step, the hydrolyzed stream goes to the saccharification and fermentation plants. First, cellulase enzymes are formed in the fermentation reactor and then the cellulase enzymes are moved to the saccharification reactor, where sugars are formed. Nutrient loadings and the efficiencies of the fermentation sugar conversion (95% for glucose, 85% for xylose and arabinose) are based on the National Renewable Energy Laboratory (NREL) process [32]. At the next step, the enzymes are recycled back to the cellulose reactor and the sugars are sent to a fermentation reactor, where ethanol is produced. The ethanol is then purified by distillation and dehydration in the ethanol recovery unit and then sent to product storage. Bottom effluent from this column contains mostly lignin from biomass and can be combusted using a combined burner, boiler and turbo-generator to produce electricity; while this electricity can be used to supply the ethanol plant, selling this byproduct is considered in our study.

3. Model Description and Data

This paper assessed the lignocellulosic bioethanol supply chain (LBSC) shown schematically in Figure 2. The supply chain consists of five layers: resources, transport, pretreatment, bioethanol production and outputs. The model equations and constraints were structured based on the LBSC flow diagram and they represent the material and energy flows from resources to products. The constraints of the model were described from use sectors back to the resources. This approach reflects the basic concept of the model, which is based on a demand-oriented analytical tool. This approach stresses the point that balance of demand and supply ought to be ascertained [33–35].

3.1. Bioethanol Production Level

Supply and demand balance is a characteristic of the model and it is guaranteed through the demand constraint expressed by Equation (1) [35]:

$$X_{C,be,\tau_C} \geq D_{be} \tag{1}$$

where D_{be} is demand for bioethanol and X_{C,be,τ_C} is exit bioethanol flow from the fermentation unit [36].

The following equation ensures the balance between inputs and outputs of the bioethanol production step:

$$X_{C,be,\tau_C} \leq X_{E,c,\tau_E} \times \eta_{C_{Ferm},c-be,\tau_C} \times \eta_{C_{Dehyd},c-be,\tau_C} \tag{2}$$

Equation (2) is a constraint which shows that the total amount of bioethanol produced from technology τ_C equals the amount of liquid delivered to the refinery from the pretreatment step, multiplied by the associated energy conversion efficiencies of the fermentation and dehydration units, $\eta_{C_{Ferm},c-be,\tau_C}$ and $\eta_{C_{Dehyd},c-be,\tau_C}$ [36].

The quantity of lignin as a byproduct of fermentation is based on inequity expressed by Equation (3):

$$X_{C,bp,\tau_C} \leq X_{T,b,\tau_T} \times x_{b,bp} \times \eta_{E,b-bp,\tau_E} \times \eta_{C,b-bp,\tau_C} \tag{3}$$

However, in addition to the fermentation step, the amount of lignin production is dependent on the type of method used for pretreatment. X_{C,be,τ_C} represents the lignin produced from cellulose to bioethanol conversion technology, X_{T,b,τ_T} is the biomass type b delivered to the preparation unit, $x_{b,bp}$ is the percent lignin for different biomasses, and $\eta_{E,b-bp,\tau_E}$, $\eta_{C,b-bp,\tau_C}$ are lignin removal efficiencies for different pretreatment techniques and conversion steps, respectively.

3.2. Pretreatment Level

The balance between the inputs and outputs of the preparation step is guaranteed by the constraint expressed by Equation (4):

$$X_{E,c,\tau_E} \leq X_{T,b,\tau_T} \times \eta_{E,b-c,\tau_E} \tag{4}$$

This equation indicates that the total amount of liquid containing cellulose extracted under pretreatment processes should equal the amount of feedstock transported to the plant, multiplied by the performance efficiency associated with different pretreatment technologies ($\eta_{E,b-c,\tau_E}$) [36].

3.3. Transport Level

The mass balance of transportation level is given by Equation (5):

$$X_{T,b,\tau_T} \leq X_{A,b} \times (1 - \iota_{T,b,\tau_T}) \tag{5}$$

where $X_{A,b}$ is the amount of biomass type b shipped from the harvesting facility to the biorefinery plant via transportation mode τ_T; ι_{T,b,τ_T} is the fraction of biomass type b lost through transportation; and $X_{T.b,\tau_T}$ represents the total amount of delivered biomass type b entering the pretreatment units [37].

3.4. Resource Level

The mass balance for the feedstocks production step is given by Equation (6):

$$X_{A,b} \leq X_{R,b} \times \varepsilon_b \tag{6}$$

where $X_{A,b}$ is the amount of waste feedstock type b that is bought from waste operators; this amount must be equal to or lower than the total waste collected by various waste companies ($X_{R,b}$), taking into account ε_b as the percentage availability of wastes.

Finally, the feasibility of biomass type b is ensured by the constraint expressed by Equation (7):

$$X_{R,b} \leq X_{0,R,b} \tag{7}$$

This equation states that the total amount of collected waste of type b ($X_{R,b}$) must be lower than the total amount of generated resource type b ($X_{0,R,b}$).

3.5. Total Material and Machinery Consumption

The total quantity of different required chemicals (CB_{b-be}) and machinery (M_{b-be}) are calculated based on Equations (8) and (9):

$$CB_{b-be}(kg) = \sum_L \sum_i X_{(L-1),b,\tau_{(L-1)}} \times cb_{L,i,\tau_L} \tag{8}$$

$$M_{b-be}(hr) = \sum_L \sum_i X_{(L-1),b,\tau_{(L-1)}} \times m_{L,b,i,\tau_L} \tag{9}$$

where $X_{(L-1),b,\tau_{(L-1)}}$ is the flow to each level L. cb_{L,i,τ_L} is the specific consumption of chemical type i (sulphuric acid, Ca hydroxide, Diammonium phosphate (DAP), cellulose, yeast) and m_{L,b,i,τ_L} is the specific consumption of machinery type i required for technology τ_L in level L. The specific consumption of different chemicals for various bioethanol production systems is shown in Table 2 [24].

Table 2. Energy and chemicals consumption through the various bioethanol production systems.

Chemicals	Units	Dilute Acid	Dilute Alkali	Hot Water	Steam Explosion
Water	m^3/ton_b	1.422	1.44	1.387	0.934
Sulphuric acid	kg/ton_b	49.04	11.40	0.00	0.00
Ca hydroxide	kg/ton_b	23.88	0.00	0.00	0.00
DAP	kg/ton_b	0.316	0.32	0.32	0.32
Cellulase	kg/ton_b	62.40	72.00	72.00	68.00
Yeast	kg/ton_b	0.79	0.79	0.79	0.79
Sodium hydroxide	kg/ton_b	0.00	0.40	0.00	0.00
Electricity	kwh/ton_b	133.44	123.50	123.28	124.00
Steam	MJ/ton_b	4870.80	4731.60	4936.80	3102.00

3.6. Potential of Bioethanol Production

The total potential of bioethanol production from various types of waste ($X_{C,b-be,\tau_C}$) is calculated by using the total amount of produced waste type b ($X_{A,b}$) and the yield of bioethanol for various feedstocks (y_{b-be}) [8]:

$$X_{C,b-be,\tau_C}(ton) \leq X_{A,b}(ton) \times y_{b-be}(\frac{ton_{be}}{ton_b}) \tag{10}$$

3.7. Modeling of Sustainability Indicators

In this section, an assessment model is presented that evaluates the sustainability impacts in the bioethanol supply chain. In the initial stages of the study, we reviewed several primary indicators

considered in [35,38,39], as well as reviewing other research works [40,41]. Finally, by consulting several studies on the energy sector, we organized five significant sustainability indicators by considering economic, energy, and environmental dimensions that cover most of the aspects mentioned by other literature on this topic.

3.7.1. Economic Indicators

Total production cost, which is the most significant economic impact for economic evaluation of bioethanol systems, is estimated by Equation (11) [35]:

$$C_{total}(\$) = \sum_{L} (C_{L,b,fix} + C_{L,b,\mathrm{var}}) \tag{11}$$

This equation includes fixed and variable setup costs for biomass type b for different supply levels of biomass production, transportation, preparation and conversion costs.

Equation (12) presents the benefit per cost (BPC), which is the ratio between sales income (from produced bioethanol and lignin) and total production costs throughout the entire bioethanol supply chain. The input costs, including capital and operational costs, and output prices for bioethanol production are provided in Table 3 [24,42–44]:

$$\mathrm{BPC} = \frac{\text{Total revenue}}{\text{Total production cost}} \frac{X_{C,be,\tau_C} \times \mathrm{Pr}_{be} + X_{E,bp,\tau_E} \times \mathrm{Pr}_{bp}}{C_{total}} \tag{12}$$

Table 3. Inputs costs and output prices in bioethanol production system.

Items	Unit	Quantity
Waste cost	\$/kg	0.014
Chemicals cost		
a. Sulphuric acid	\$/kg	0.035
b. Ca hydroxide	\$/kg	0.1
c. DAP	\$/kg	0.21
d. Cellulase	\$/kg	0.52
e. Yeast	\$/kg	2.3
f. Sodium hydroxide	\$/kg	0.45
Water cost (usage fee)	\$/m^3	0.32
Energy cost		
a. Electricity	\$/kwh	0.03
b. Truck diesel	\$/L	1.08
Capital cost of bioethanol production by using:		
a. Dilute acid	\$/ton_b	457.52
b. Dilute alkali	\$/ton_b	410.93
c. Hot water	\$/ton_b	407.78
d. Steam explosion	\$/ton_b	363.45
Product price		
Bioethanol	\$/kg	0.85
Lignin	\$/kg	0.25

3.7.2. Energy Indicators

All stages of the bioethanol production process are based on the consumption of specific sources; therefore, to properly assess energy inputs and outputs, it is necessary to convert all inputs and outputs

into their energy equivalents. The energetic efficiency of the bioethanol system is evaluated by the energy ratio between outputs and inputs as shown in Equation (13) [35,45]:

$$\text{EUE} = \frac{\text{Total output energy}}{\text{Total input energy}} = \frac{X_{C,be,\tau_C} \times ec_{be} + X_{E,bp,\tau_E} \times ec_{bp}}{\sum_L \sum_{in} u_{L,b,in,\tau_L} \times ec_{in}} \quad (13)$$

where bioethanol and lignin are considered as output energies and water, fuel, power, chemicals and machinery demand energy input type *in* in supply level *L* for bioethanol production u_{L,b,in,τ_L}). A comprehensive inventory of various inputs for the whole system, based on the studied pretreatment methods, is gathered with the energy coefficients for all inputs (ec_{in}) in Table 4 [24,45].

Table 4. Energy coefficients for different inputs and outputs to the bioethanol production system.

Input	Unit	Energy Coefficient (MJ/unit)
Diesel fuel	L	47.80
Electricity	kWh	11.93
Chemicals and machinery in bioethanol production	ton_b	37.5
Bioethanol	kg	29.3
Lignin	kg	21.13

3.7.3. Environmental Indicators

Greenhouse gas (GHG) emissions are one of the most significant environmental indicators, representing the emissions of the major greenhouse gases (CO_2, CH_4 and NO_2) during the unit life cycle. In this study, total GHG emissions over the bioethanol production cycle is calculated by Equation (14) [35]:

$$\text{GHG } (kgCO_2eq) = \sum_L \sum_{in} u_{L,b,in,\tau_L} \times ef_{in} \quad (14)$$

where u_{L,b,in,τ_L} is the required input type *in* for bioethanol production from biomass *b* in level *L* based on technology τ_L, and ef_{in} are the CO_2 emission factors for different inputs; this factor is considered 2.76 $kgCO_2eq/L$ and 0.058 $kgCO_2eq/kWh$ for diesel fuel and electricity generated from geothermal, respectively. Moreover, during fermentation, sugars are converted to ethanol and carbon dioxide. Approximately, 720 kg CO_2 is produced per ton of bioethanol produced [21,46,47]. Firstly, in hydrolysis the cellulose is converted into glucose sugars. Then, sugars are converted to ethanol and carbon dioxide [48].

To facilitate a fair comparison between bioethanol systems, water used over the entire system (W_{b-be}) is measured by the water consumption indicator expressed by Equation (15) [35]:

$$W_{b-be}(m^3) = \sum_L X_{L,b,\tau_L} \times w_{L,b,\tau_L} \quad (15)$$

where X_{L,b,τ_L} is the exit flow from level *L* based on technology type τ_L and w_{L,b,τ_L} is the specific water consumption for each level and technology (which are given in Table 2).

4. Results and Discussion

4.1. Economic Assessment

The model results for the 12 alternatives, ranked according to their contribution to production costs and benefit per cost for 1 ton of bioethanol produced, are shown in Figure 3. This ordering is based on total production cost, which is between 1300 and 2700 $/ton, which are the highest and lowest economically beneficial options, respectively. Moreover, the coloured portions of each bar on the chart indicate the percentage impact of each type of cost for different bioethanol supply levels (BC: biomass cost, TC: transportation cost, CC: conversion cost including pretreatment, fermentation

and dehydration costs). Obviously, TC is much lower than the other levels and hence is not shown clearly in Figure 3.

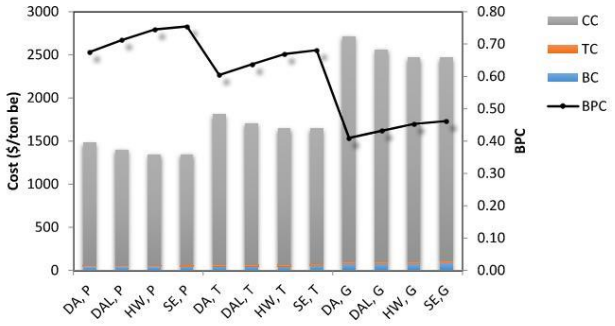

Figure 3. Production costs and BPC for 1 ton bioethanol produced from different wastes; BPC: benefit per cost, BC: biomass cost, TC: transportation cost, CC: conversion cost.

Among the studied wastes, paper and paperboard rank the highest economically; the average total cost of bioethanol production from timber and wood and garden waste is 1.2 and 1.9 times that of paper, respectively. Actually, the higher cellulose percent in lignocellulosic materials means more bioethanol yield can be obtained. In contrast, for a specific amount of bioethanol production, a lower feedstock with a high percentage of cellulose is required. The cellulose percentage of paper, timber and garden wastes are approximately 55%, 45% and 30%, respectively [49,50]. Thus, paper waste is the richest in cellulose and thus has the minimum feedstock requirements for 1 ton of produced bioethanol (Figure 4). Subsequently, this option has the lowest percentage of costs from biomass and transportation due to the lower amount of required feedstock and the higher bioethanol yield. In this way, the costs of waste purchase and transportation for timbers and garden wastes are approximately 1.20 and 1.85 times that for paper.

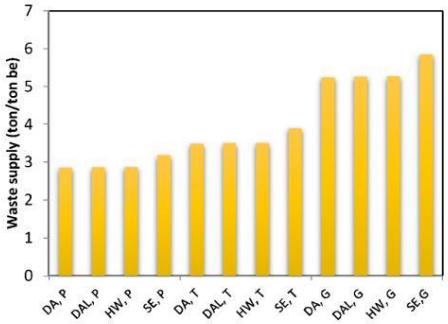

Figure 4. Waste required to produce 1 ton bioethanol; P: paper and paperboard, T: timber and wood, G: garden waste, DA: dilute acid, DAL: dilute alkali, HW: hot water, SE: steam explosion.

As seen in Figure 4, the bioethanol system derived from paper via steam explosion (SE,P) significantly outranks all other systems from the viewpoint of BPC, owing to the favorable results obtained in the economic sector. Although the ethanol yields for steam explosion were relatively low (0.39, 0.32 and 0.21 L_{be}/ton_b for paper, timber and garden wastes, respectively) due to the

comparatively low efficiency of cellulose hydrolysis, it has the lowest capital costs because of the high solid loading assumptions during pretreatment and hydrolysis processes. Furthermore, no chemicals are required for SE pretreatment and it requires the lowest amounts of steam and electricity for its various processes.

4.2. Energy Assessment

Total input energy, total output energy and energy ratio between outputs and inputs (EUE) for 1 ton of bioethanol produced are shown in Figure 5. The total output energy for various feedstocks includes the energy content in 1 ton of bioethanol and lignin production. Obviously, due to the higher required amount of timber and garden waste, more lignin is produced. Significantly, the system based on steam explosion and paper ranks the highest among all the systems in terms of energy. This is because no chemicals except water are required in SE and the smallest amount of steam is consumed during this process. On the contrary, the dilute acid method, which requires 1.08 and 1.6 times the amounts of heat and electricity required for SE, also has the highest usage of chemicals and is ranked lowest energetically.

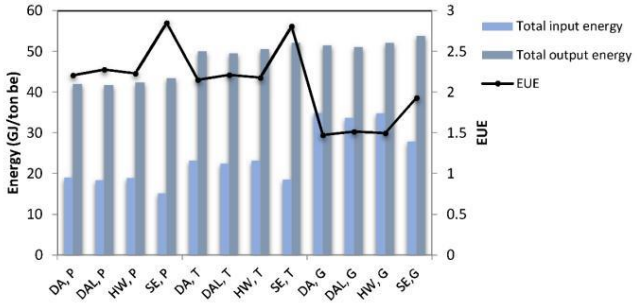

Figure 5. Total input energy, total output energy and EUE for 1 ton bioethanol production from different wastes.

4.3. Environmental Assessment

Figure 6 ranks all the studied bioethanol systems with regard to their contribution to environmental development. This ordering is based on total GHG emission, which is lowest for the steam explosion and hot water processes (about 880 $kgCO_2eq/ton$). The environmental impact of SE and HW are additionally limited because few chemical agents are used in these methods.

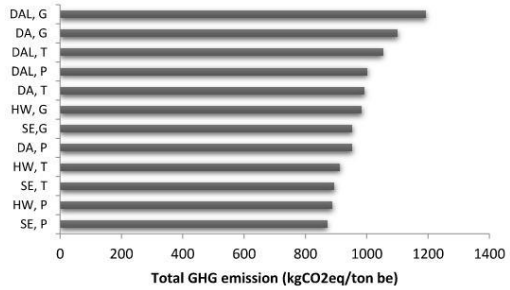

Figure 6. Total GHG emission for 1 ton of bioethanol produced by using different wastes.

Figure 7 shows total water consumption over the entire waste-to-bioethanol process for all the production options. The systems based on steam explosion and paper and timber have the lowest water use, 2.98 and 3.64 m^3/ton, respectively. According to Kumar and Murthy [24], the amount of water required for cooling is lowest for the steam explosion process (401.4 kg/L of ethanol) due to higher solid loading, which decreases the flow rates of streams and energy consumption for cooling. Moreover, bioethanol systems based on dilute alkali and dilute acid for garden wastes require the maximum amounts of water. Obviously these systems would not be practical for regions lacking sufficient available water resources.

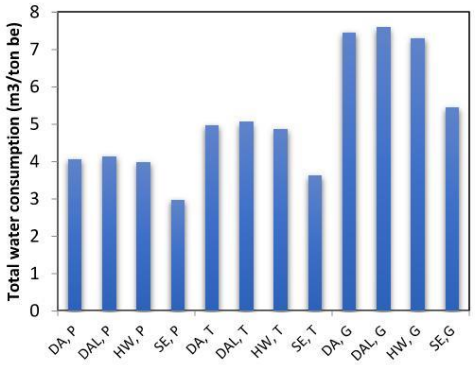

Figure 7. Total water consumption for 1 ton of bioethanol produced by using different wastes.

4.4. Potential of Bioethanol Production

The potential of different wastes and bioethanol production between 2015 and 2030 are shown in Figure 8. The data presented here are drawn from [8]. The main sources of paper and paperboard waste that are suitable for bioethanol production are newspapers, magazines and packaging waste. In addition, the main sources of timber waste are timber from construction, demolition work, packaging waste and pallets. Garden waste can be also defined as grass, branches and other garden waste.

The total amount of paper, timber and garden wastes in Iceland in 2015 can be estimated as approximately 37, 40 and 16 thousand tons, respectively, and they can estimated to increase to about 47, 49 and 20 thousand tons by 2030 assuming 0.8%, 0.6% and 0.6% growth rate per capita, respectively.

Furthermore, Figure 8 shows predictions of ethanol production from various feedstocks. This calculation is based on the average yield of bioethanol production (Equation (10)) calculated as 339, 277 and 185 (kg_{be}/ton_b) for paper, timber and garden wastes, respectively. The average potential of bioethanol production in Iceland in 2015 was thus approximately 12.5, 11 and 3 thousand tons from paper, timber and garden wastes, respectively, which may reach about 15.9, 13.7 and 3.7 thousand tons by 2030.

Moreover, the potential of bioethanol production employing different pretreatment technologies and various MOWs in 2015 is depicted in Figure 9. It is observed that maximum ethanol production is possible using dilute acid, dilute alkali, hot water and steam explosion. Ethanol yield is relatively low for the steam explosion system due to its comparatively low efficiency of cellulose hydrolysis.

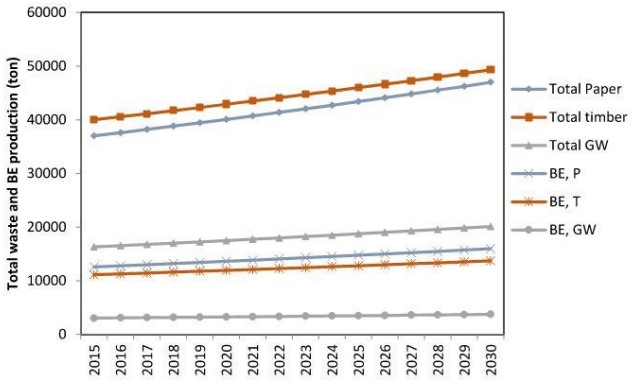

Figure 8. Total amount of various wastes and bioethanol production between 2015 and 2030.

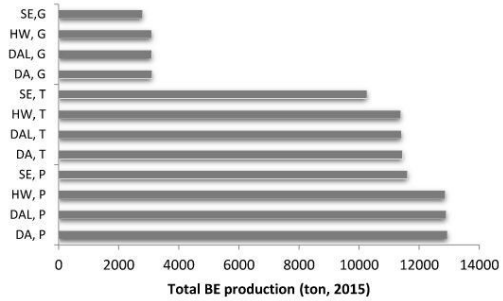

Figure 9. Total bioethanol production in 2015.

4.5. Comparison of Alternatives

The rank orders for the 12 alternative bioethanol systems considered herein across the studied sustainability indicators are shown in Table 5.

Table 5. Rank order of bioethanol systems based on sustainability indicators.

Systems	BPC	EUE	GHG Emission	Water Consumption	Production Yield
SE,P	1	1	1	1	4
HW,P	2	4	2	3	3
DAL,P	3	2	9	5	2
DA,P	5	5	5	4	1
SE,T	4	3	3	2	8
HW,T	6	7	4	6	7
DAL,T	7	6	10	8	6
DA,T	8	8	8	7	5
SE,G	9	9	6	9	12
HW,G	10	11	7	10	11
DAL,G	11	10	12	12	10
DA,G	12	12	11	11	9

SE,P is the top ranked system for nearly all impact indicators, except for production yield, for which it is in fourth place. DA, DAL and HW for garden wastes have the lowest ranks for almost all of the indicators. In addition to SE,P, more economic and environmentally oriented policies should favor HW,P and SE,T. Moreover, DAL,P ranks high for most indicators except for environmental, due to its high GHG emissions and moderate water consumption. DA,P has ranks low for most of the indicators, except for technically occupying the highest position for production yield. Finally, among the MOWs, paper and paperboard rank highest in most assessments.

5. Conclusions

This study presented a comprehensive sustainability assessment model covering the entire lifecycle of bioethanol production (resources, transport, pretreatment and production) to produce lignocellulosic bioethanol from various types of MOWs in Iceland: paper and paperboard, timber and wood and garden waste. Moreover, we carried out an analysis and comparison of the 12 systems based on sustainability impacts (economic, energy, environmental and technical) using the most common pretreatment technologies: dilute acid, dilute alkali, hot water and steam explosion. Based on the analysis conducted, the following conclusions can be reached:

(1) Among the MOWs, paper and paperboard rank highest in most assessments. The steam explosion option is the most beneficial production technology from an economic, energy and environmental perspective; thus, it would be the most promising technique for producing bioethenal from the studied wastes.

(2) The dilute acid method also ranks highly, technically; however, this it is not a desirable option due to its low energy performance, high production costs and high greenhouse gasses emission.

(3) In addition to steam explosion, more economic and environmentally oriented policies should favor hot water technology, as no chemicals are required for treatment and the hydrolysis yield is similar to that of other pretreatment methods.

(4) The dilute alkali technique for deriving bioethanol from paper also ranks highly for most of the indicators, except for environmental, due to its high GHG emissions and moderate water consumption.

(5) Finally, estimates of the potential of different wastes and bioethanol production types in 2015 and 2030 were calculated. The total amount of paper, timber and garden wastes in Iceland in 2015 can be estimated as approximately 37, 40 and 16 thousand tons, respectively, which could increase to about 47, 49 and 20 thousand tons by 2030. Thus, the average potential of bioethanol production in 2015 was approximately 12.5, 11 and 3 thousand tons from paper, timber and garden wastes, which may likewise increase to about 15.9, 13.7 and 3.7 thousand tons in 2030.

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Paper II

A review of biomass gasification modelling.
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A review of biomass gasification modelling

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ABSTRACT

Currently around 10% of all energy generated worldwide comes from biomass. Most of this 10% is biofuel energy from the fermentation of corn and sugarcane. Fermentation of corn competes with the global food supply, and fermentation of sugarcane drives deforestation. Therefore, the renewable and sustainable growth of these two bio-based energy sources may not be desirable even if it is economically feasible. Biomass gasification by contrast is significantly more flexible in terms of the bio-feedstock or waste that can be processed to either produce biofuels or to co-generate electricity and heat on demand. Fluidized bed and entrained flow gasifiers already achieve promising economy-of-scale for fuel production whilst downdraft gasifiers are well-suited for small-scale heat and power co-generation. This superior flexibility of gasification both in terms of the feedstock type and also the energy generation or fuel production options, is what drives expanding research and implementation opportunities for biomass gasification. Research progress is accelerated by modelling work. This review is the first review in the biomass gasification modelling field to collect and analyze statistics on the growing number of gasification modelling studies and approaches used. The frequency of the various modelling choices made, and the trends this data reveals, is reported. For new researchers this review provides a succinct guide to the modelling choices that needs to made early on in a modelling study or project. A detailed methodology characterization is introduced that includes consequential modelling choices not explicitly addressed by prior reviews. To seasoned researchers this study provides the first statistical (as opposed to ad hoc or anecdotal) picture of what their fellow researchers are doing.

1. Introduction and objectives

Currently, about 81.4% of the world's primary energy requirements are supplied by the big three fossil fuels (oil, coal and natural gas). The next biggest contribution, approximately 9.7%, is derived from biomass (primarily ethanol and biodiesel) and waste. The remainder of the world's energy needs is supplied by nuclear (~4.9%), hydroelectric (~2.5%) and the trio of rapidly growing renewables geothermal, solar and wind that currently account for ~ 1.5% [1–3].

Using fossil fuels to produce energy has negative social, political, and environmental impacts, and the burning of fossil fuels has increased global CO_2 concentrations and further intensified climate change [4–8]. These consequences are strong motivators for the development of renewable and domestically available energy sources [9]. Among the various renewable energies, biofuels from biomass have seen large-scale implementation (especially sugarcane ethanol in Brazil and corn ethanol in the US) as transportation fuels, allowing for more fuel security and the creation of new job opportunities. As can be seen from the world energy statistics in the opening paragraph biofuel and waste already are surprisingly large source of the world energy supply with the waste-to-energy sector growing and developing rapidly [7,10].

Recovering energy from biomass or organic solid waste requires biochemical and/or thermochemical processes [11]. During biochemical processes like fermentation, biomass is converted to biofuels through the digestive action of living organisms. However, in thermochemical processes, biomass is converted to biofuels, gases, and chemicals by applying heat and/or pressure. Gasification, also widely used to gasify coal and natural gas, is the most prominent thermochemical biomass-to-energy and waste-to-energy conversion processes gaining ever more research and commercial interest [10]. In addition to producing syngas from biomass for subsequent biofuel synthesis, gasification typically achieves superior efficiency for electricity generation compared to more conventional alternatives such as incineration (to generate steam for turbines). Electricity production utilizing gasification recover more electricity per kilogram of biomass [12] or per kilogram of municipal waste [13–15] compared with alternatives such as incineration or biogas from digesters. Using gas engines, gas turbines or fuel cells, electricity can easily be generated from syngas with existing or marginally modified infrastructure. In certain situations, the superior energy recovery efficiency of gasification does result in the

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lowest cost (compared with conventional technologies) in per unit of energy produced from biomass [12,16]. Hence, the thermochemical or gasification route between raw biomass and energy is significantly more flexible than the currently dominant biochemical route – predominantly the fermentation of corn or sugar cane to ethanol. Gasification can economically transform many more types of biomass compared to fermentation. Demonstrated feedstock include most types of organic waste, sea-weed and forestry waste. The syngas produced from any of these sources is readily processable into liquid fuels or can fire the efficient co-generation of heat and electricity. It is on account of this superior flexibility of gasification, both on the feedstock end and energy generation end, that gasification will likely play an ever increasing role in our future energy mix.

The performance of the process can be influenced by many factors, including feedstock, process design, and the operating parameters [17]. As a result, gasifier reactors need to be designed either by experimental data and/or by using mathematical or simulation based modelling of the gasification process. The experimental option, though the most reliable, is best utilized in combination with modelling [18]. In practice modelling always play a key role both in applied gasification R&D work or in more fundamental research studies. When it comes to the applied work models that are validated through experiments do reliably predict gasifier performance as a function of feedstock and give qualitative and quantitative information for prospective practical operations. Modelling is very effective in optimizing the operation of an existing gasifier, as well as in exploring operational limits and gaining insight into the relationship between operational parameters and in explaining trends in the data [19]. Simulations also serve as a low-cost method for exploring the potential benefits, costs, and risks associated with the implementation of gasification given the fact that time and budgets for experimentation and pilot data collection are always finite [18].

When it comes to more fundamental research aimed at understanding mathematical models and simulations have been used extensively as well by researchers and equipment manufacturers. Moreover, only the combination of experiments and process modelling can provide an understanding of the physical and chemical phenomena within the gasifier.

However, the range of complexity and detail that can be included, or omitted, in any gasifier model is large. A detailed fine-grained simulation of the gasification process involves the modelling of heat and mass transfer, multiphase fluid dynamics, chemical transport and multiple heterogeneous and homogenous chemical reactions. Both applied and scientific modelers need to make a large number of choices regarding modelling type and what to include and what to omit or approximate.

By now, there is a substantial body of literature utilizing models of various types of gasifiers that have different degrees of complexity. However, reviews of these modelling and simulation studies are somewhat limited [18]. Our review found seven other reviews, which may sound sufficient if not for the fact that there is a significant amount of repetition among several of them [18,20–25]. There is a particular need for reviews that are not just a catalogue of types of models and prior studies but that instead systematically compare modelling approaches and answer important questions about what is known about the relative merits of these modelling approaches. For example, the current review is the first to address whether or not stoichiometric and nonstoichiometric models lead to identical predictions or not. The present review is also the first to consider the more consequential choices that a modeler has to make, namely whether to use a total equilibrium or semi-equilibrium approach (see section 4). Another feature of the current study that differs from prior reviews is the inclusion of representative statistics indicating the frequency of the use of the various competing modelling choices in the literature to date.

Finally, the existing review articles do not address the recent progress made in the area of tar modelling. The results of the current review confirm that the vast majority of gasification models and simulations treat tar in gasification in one of three ways, namely as either not present in the gas phase (i.e. absent or negligible), present but inert, or where all tar species are modeled by a single (or a couple of) representative model compound(s) (with aromatics such as benzene or naphthalene, the most typical choices) [26]. Of course, all three options are a vast oversimplification, but in all three cases, the vital question to the researcher or engineer is how large the error incurred is with a given simplification in a given application. In the past, it is likely that these simplifications were primarily motivated not by the certain knowledge that the error incurred was acceptably small, but rather by the fact that tar is complex, and its composition and reactivity varies according to the process operating conditions [27]. Furthermore, the experimental characterization of the tar species present within and during gasification is very limited, which is in part because of the difficulty of sample extraction and analysis [21]. A review that includes a survey of what is known about the answer to these questions in various scenarios should be practically useful. In addition, for those scenarios where a more sophisticated tar treatment would make a worthwhile or critical difference, new tar models and treatment approaches have been developed in recent years [21,26,28] These tar models are included in the current review. In the present work, a comprehensive study of the developed models and a new classification of the most important gasification modelling approaches is introduced. Frequency of use statistics is presented. Finally, tar modelling and its approximation methods are surveyed.

2. Methodology of article selection

This section describes the systematic search strategy (outlined in Fig. 1) followed to select articles for inclusion in the statistics and discussion in this review. As a starting point three databases, namely Google Scholar, Ardabil Science and Science Direct were searched for keywords gasification and modelling or modelling. This search strategy yielded 457 results. After removing duplicates and any review articles, the total dropped to 421 works. The next step is to identify and filter out and retain just articles with focus on, overlap with, or relevance to biomass gasification. Screening the articles with these criteria revealed 156 publications that met the criteria based on their titles and abstracts and another four articles were provisionally included after screening the references of the relevant articles by hand. Further assessment of eligibility based on full-text works led to 54 studies being selected, with

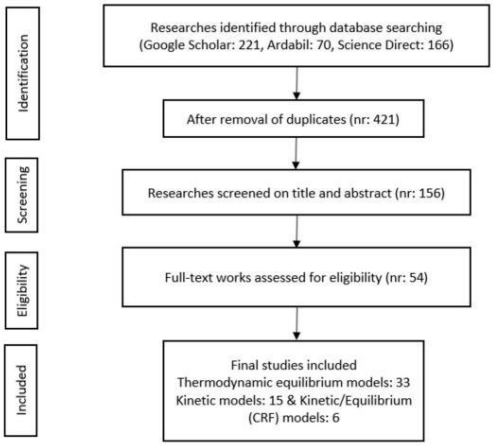

Fig. 1. Flow diagram depicting the details of the literature search.

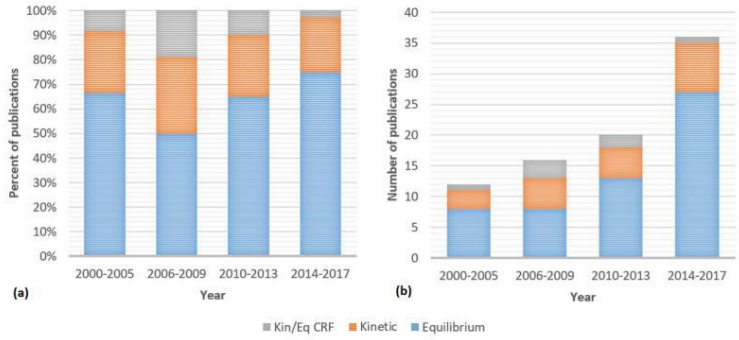

Fig. 2. Overview of gasification models since 2000, (a) as percent, (b) absolute number of studies.

33 studies on thermodynamic equilibrium models, 15 works on kinetic modelling, and 6 studies on kinetic/equilibrium (CRF) modelling. One aim of the current review was to provide a better understanding of the prevalence of these approaches. The relative prevalence of these main modelling approaches over time is shown in Fig. 2 [11,17,26,29–94]; in Fig. 2, it can be seen that thermodynamic equilibrium modelling has been favored to date and is currently the chosen approach in roughly 60% of models and simulations published to date. What our survey suggests, perhaps for the first time, that equilibrium models are perhaps not just chosen because of a lack of kinetic data, as is sometimes assumed. This conclusion is suggested by the fact that our statistics show that although the amount of mechanistic and kinetic data has grown steadily since 2006, the fraction of simulation and modelling studies that chose kinetic over equilibrium models has not grown together with the availability of kinetic data. In fact, the fraction of modelling studies that use equilibrium only approaches have actually increased from a low in the period 2006–2009 (around 50% of models) to being the chosen modelling approach in about 75% of biomass modelling articles from 2014 to 2017.

3. Gasification process and technologies

3.1. Gasification process overview

Gasification is the conversion of solid or liquid feedstock into syngas. The syngas is used as a chemical feedstock or is utilized directly as a fuel to generate heat, electricity, or both. The gasification process consists of the following stages: drying, pyrolysis, oxidation (combustion), reduction (char gasification), and cracking (Fig. 3) [95].

Typically, the moisture in the biomass feed ranges from 5 to 35% that during drying step, it is reduced to below 5%. In the pyrolysis step, the biomass is heated from 200 up to 700 °C with limited oxygen or air. Under these conditions the volatile components in the biomass are vaporized. The volatile vapor is a mixture of hydrogen, carbon monoxide, carbon dioxide, methane, tar (heavier hydrocarbon) gases, and water vapor [96]. Tar (a black, viscous, and potentially corrosive liquid at standard temperature and pressure that is predominantly composed of heavy organic and inorganic molecules) and char (a solid residue mainly containing carbon) are also produced during pyrolysis [97]. The oxygen supplied to the gasifier reacts with the combustible substances, producing CO_2 and H_2O. Some of this CO_2 and H_2O subsequently are reduced to CO and H_2 upon contact with the char produced from pyrolysis [19]. Moreover, the hydrogen in the biomass can be oxidized, generating water. The reduction reactions occurring inside the gasifier are endothermic, and the energy required for these reactions is provided by the combustion of char and volatiles. Reduction of the biomass yields combustible gases such as hydrogen, carbon monoxide, and

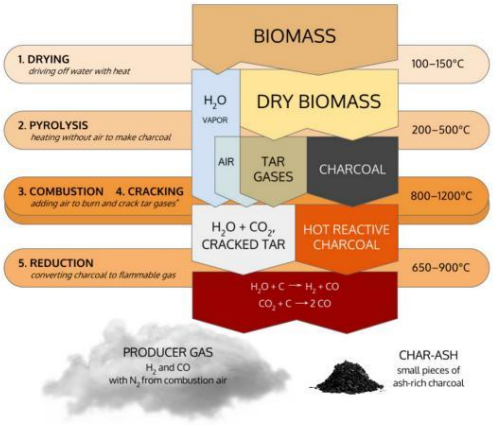

Fig. 3. Gasification process steps (Reprinted from www.allpowerlabs.com, Copyright 2018 All Power Labs, with permission from All Power Labs).

methane through a series of reactions; the main reactions in this category are as follows [20,97]:

Moreover, the tar gases produced during the pyrolysis step undergo cracking in the gasification step, which produces a mixture of non-condensable gasses, light hydrocarbons, and unconverted tar. This process is represented by equation (1), with γ showing the yield coefficients of the product gasses and unconverted tar. The values of the γ coefficients depend strongly on gasifier operating parameters and feedstock type. However, it is treated as a constant in some works [26]. The most important parameters determining the γ coefficients are temperature, pressure, gasifying medium, catalyst and additives, equivalence ratio (ER), and residence time.

$$tar \rightarrow \gamma_{CO} CO_{(g)} + \gamma_{CO_2} CO_{2(g)} + \gamma_{CH_4} CH_{4(g)} + \gamma_{H_2} H_{2(g)} + \gamma_{tar_{inert}} tar_{inert} \quad (1)$$

An example of a relatively more detailed account of tar cracking, steam and dry reforming, and carbon formation was developed by Devi et al. [27]. Their model utilizes the following reactions:

Cracking: $pC_nH_x \rightarrow qC_mH_y + rH_2$ (2)

Steam reforming: $C_nH_x + nH_2O \rightarrow (n + {}^{x}/_{2})H_2 + nCO$ (3)

Dry reforming: $C_nH_x + nCO_2 \rightarrow (^{x}/_{2})H_2 + 2nCO$ (4)

Carbon formation: $C_nH_x \rightarrow nC + (^{x}/_{2})H_2$ (5)

where C_nH_x represents tar and C_mH_y represents dehydrogenated hydrocarbons.

Endothermic reactions decrease the temperature in the reduction zone and the temperature further falls downstream from the gasifier. As a result, most of the tar condenses out in these segments. The resulting tar deposits block and foul engines and turbines, downstream reactors, the syngas conditioning and filtration system. Several efficient methods have been employed to achieve tar removal from the outlet gas. Tar removal technologies can be divided into two approaches: hot gas cleaning after the gasifier (secondary methods) and treatments inside the gasifier (primary methods). Secondary techniques are conventionally used for the treatment of the hot product gas from the gasifier. Tar reduction can be achieved either chemically by using a catalyst or physically by using a cyclone, baffle filter, ceramic filter, fabric filter, rotating particle separator, electrostatic filter, or scrubber. In the primary treatment, the gasifier is optimized to produce a product gas with minimum tar concentration. The different primary treatment approaches are (a) the appropriate selection of operating parameters, (b) use of a bed additive or catalysts, and (c) gasifier modifications. The operating parameters such as temperature, gasifying agent (e.g., air, pure steam, or steam–O_2 mixtures), ER, and residence time play an important role in tar formation and decomposition. By using some active bed additives such as dolomite, olivine, or char inside the gasifier, it is possible to improve the gasifier's performance.

As mentioned, in the pyrolysis step, heat provided by combustion heats the dry biomass to the point that it decomposes into solid char and volatiles (tar and gases). The sum of the tar and gases are equal to the volatile matter (VM), the amount of which is typically quantified using a proximate analysis [26]. The VM percent for different kinds of woody biomasses is high relative to coal, with biomass VM typically in the range of 70–90% by mass. Moreover, char is often modeled as consisting of carbon only, and its amount would be equal to the fixed carbon extracted from the proximate analysis [56]. The typical mass fraction division of the streams within the pyrolysis and gasification steps is depicted in Fig. 4. The mass flow distribution in this illustrative example are based on the gasification of Olive Wood in a fixed bed downdraft gasifier with air as agent, as reported by Ref. [31]. It can be seen that in this particular case, well more than 90% of a downdraft gasification input mass end up in the syngas product stream, while the final tar content in our example is about 0.1% (in general it ranges from 0 to 5%) of the inserted wood material. Hence, the tar amount can be almost negligible in many applications especially if pyrolysis tar is combusted, cracked and reduced.

Pyrolysis of biomass and wood gasification produce about 10–30 wt % char and tar in (e.g. Ref. [98]). The 10 wt% char and 5 wt% tar produced from olive wood pyrolysis reported by Ref. [31], which is shown in Fig. 4, may be on the low end. The amount of tar that exits either with the product gas, or condenses out on downstream components, depends significantly on the gasifier type and operating conditions and even factors such as the amount of char present in the reduction zone (which can be catalytic for tar cracking and reduction [98–100]). For example, Baker et al. conducted an early survey that found tar yield up to 12 wt% for some updraft gasifiers and in the range of 4–15 wt% for fluidized bed gasifiers, with the higher end observed at lower temperatures (600 °C) [100]. Downdraft gasifiers operating at a relatively higher temperature of 900 °C tend to perform well in terms of final tar yield, with a final tar yield less than 1 wt% common [31,100].

3.2. Gasification technologies for biomass

Gasifiers can be divided into two principal types of fixed beds and fluidized beds.

- Fixed-bed (updraft, downdraft, cross-draft): The fixed-bed gasifier category includes gasifiers with a bed filled by solid fuel particles where the gasifying media and gas either are rising (updraft), descending (downdraft), or flowing horizontally through the reactor (cross-draft) [20]. The gasifying media may be air, steam, oxygen, or a mixture of them. The two main practical advantages of fixed-bed gasifiers are that they are relatively more cost-effective for small-scale applications and tend to produce a clean product gas with low dust and low tar content when compared with fluidized bed alternatives [101]. The main disadvantage is that they can have poorer heat transfer and temperature inhomogeneity, and they do not scale up as well as fluidized bed gasifiers. Secondly, fixed-bed gasifiers typically require tighter feed specifications – for example a moisture level below 20% and a fairly uniform particle size distribution with few fines for the biomass (to prevent clogging and channeling).
- The fluidized bed (bubbling, circulating): A typical fluidized bed is a cylindrical column that contains particles and through which fluid—either gaseous or liquid—flows. The velocity of the fluid is sufficiently high enough to suspend the particles within the column, providing a large surface area for the fluid to make contact with, which is the chief advantage of fluidized beds. The main potential advantages of fluidized beds are their superior heat and material transfer between the gas and solid phases. Thus, a fluidized bed maintains a homogeneous temperature field and is more flexible in the sense of wide variations in fuel quality. The main downside of fluidized bed gasifiers is that they tend to produce more dust and particulates in the product gas, which can present a significant problem for downstream equipment [102].

Among these gasifier types fluidized bed gasifiers and entrained flow gasifiers (due to scalability and the related specific investment cost required for the downstream gas cleaning and chemical synthesis) currently appears the most promising candidates for biofuel production plants. For small-scale distributed power production downdraft gasifiers has emerged as typically the most suitable option among gasifier types.

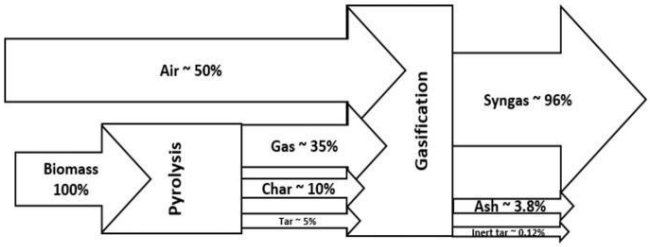

Fig. 4. A Sankey chart of mass flow distribution throughput biomass gasification.

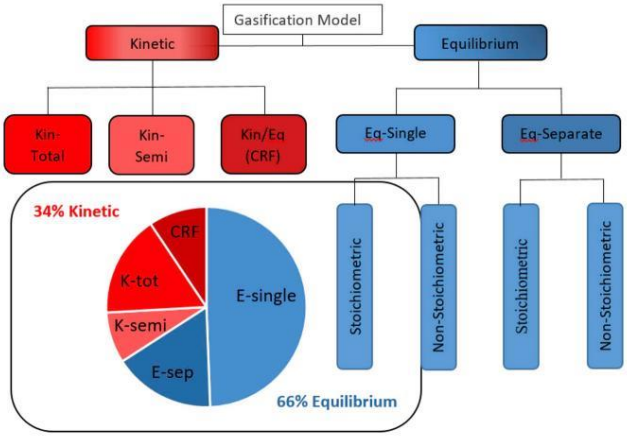

Fig. 5. A categorization of gasification model types.

4. Biomass gasification models

The main two categories of gasification models are equilibrium and kinetic models. This survey of gasification modelling choices found that roughly 66% biomass gasification simulations utilize some type of eq equilibrium model, and the remaining 34% utilize some type of kinetic model (see Fig. 5). This section will discuss the main variations of both these approaches, but first a brief review of reasons for modelling and simulating biomass gasification are studied. Moreover, features and weakness of these methods are gathered in Table 2 [18,20,24].

A gasification plant operator needs to optimize the feedstock flow rate, agent flow rate, equivalence ratio, reactor pressure, and temperature to achieve a desirable syngas composition and yield. Changes in any of these parameters can have a substantial impact on the product compositions and the gasifier performance [24]. Moreover, the admissible range for feedstock properties is rather narrow because the chemistry and fluid dynamics of gasification are very sensitive to variations in feedstock composition, moisture, ash content, particle size, and density [24]. In practice, laboratory experiments, pilot facilities, and field experience can and do provide information regarding the optimum conditions and appropriate feedstock for a reactor, but these lessons can be more time-consuming and expensive compared with modelling.

A higher degree of insight and economic efficiency can be obtained by combining mathematical modelling and process simulation with physical experimentation. A good model should give a reasonably accurate representation of the chemical and physical phenomena occurring inside the gasifier reactor. One approach to ensure the predictive ability of a model is to strive to include all reactions and transport phenomena as realistically as possible. However, in practice, modelers invariably must ignore some of the details and make simplifying assumptions that decrease the complexity of the model. Thus, practically all models inevitably will be approximations, and the question is just how good of an approximation a given model is. A good example of the unavoidable need for simplification is tar formation and cracking. The number of detectable hydrocarbon species within a tar sample, and the number of relevant formation, conversion reactions can be in the hundreds [21]. As a result of this complexity, many models ignore tar modelling altogether. In our survey just under 12% of all published biomass gasification simulations included any tar modelling. Notwithstanding the fact that minimizing tar is a practically and operationally important objective—tar either condenses out in the downstream equipment and reducing its performance, or pollutes the product syngas. Whenever tar is included, it is always in a simplified form compared to reality.

Table 1
Main gasification reactions [20,97].

Heterogeneous reactions		
$C + O_2 \rightarrow CO_2 + 394$ kJ/mol	Complete combustion	R1
$C + 0.5O_2 \rightarrow CO + 111$ kJ/mol	Partial combustion	R2
$C + CO_2 \rightarrow 2CO - 172$ kJ/mol	Boudouard	R3
$C + H_2O \rightarrow CO + H_2 - 131$ kJ/mol	Water-gas	R4
$C + 2H_2 \rightarrow CH_4 + 75$ kJ/mol	Methanation	R5
Homogeneous reactions		
$CO + 0.5O_2 \rightarrow CO_2 + 283$ kJ/mol	CO partial combustion	R6
$H_2 + 0.5O_2 \rightarrow H_2O + 242$ kJ/mol	H_2 combustion	R7
$CO + H_2O \rightarrow CO_2 + H_2 + 41$ kJ/mol	Water-gas shift (WGS)	R8
$CH_4 + H_2O \rightarrow CO + 3H_2 - 206$ kJ/mol	Reforming	R9
H_2S and NH_3 formation reactions		
$H_2 + S \rightarrow H_2S$	H_2S formation	R10
$3H_2 + N_2 \rightarrow 2NH_3$	NH_3 formation	R11

4.1. Thermodynamic equilibrium models

The thermodynamic equilibrium approach predicts the composition of the outlet gases based on the assumption that the components react in a fully mixed condition for an infinite period of time [24,25]. A less strict—and more practical—definition of the set of assumptions that would justify the use of an equilibrium modelling approach in a real gasifier is when the following conditions are met:

1) Reactant residence time (τ_{res}) in the reduction zone is long compared to the half-life ($\tau_{1/2}$) of all reactants. In essence $\tau_{res} \gg \tau_{1/2}$, with $\tau_{1/2}$ a time scale determined by the reaction rates of the rate limiting reaction (s),
2) the temperature in the reduction zone can be assumed as constant, and
3) chemical mixing is close to perfect.

Thermodynamic equilibrium calculations are simple compared with kinetic models and independent of the gasifier design, and in the simplest, most ideal case, general thermodynamic properties can be used for equilibrium modelling, while a larger set of hard-to-come-by and accurate kinetic parameters is needed for kinetic modelling. These

Table 2
Features and weakness of gasification modelling approaches.

	Features	Weakness
Equilibrium modelling	• Simple method • Not required to consider chemical reactions • Useful tool to evaluate a complex reacting system that is difficult or unsafe to produce experimentally or in commercial operation • Predicts the maximum achievable yield of the products • Very useful in the predicting of downdraft gasifiers • Useful tool for a preliminary comparison of fuels and process parameters • Independent of gasifier design • Flexible for various feedstocks and process parameters • Good representation for high temperatures (750–1000 °C) • Can be improved by using the coefficients for equilibrium constants or yields distribution	• Assumption that the components react in a fully mixed condition for an infinite time period • Assumption that the reactor is zero dimensional • Tars are not considered • Heat loss is neglected • Not fully attained for low operation temperatures • Limitation is for fluidized bed gasifiers • Cannot give highly accurate results for all cases
Kinetics modelling	• Consideration of finite time or finite volume • Accurate and detailed results • Good approximation at low temperatures • Includes both reactions kinetics and hydrodynamics inside the gasifier • Very useful tool for the evaluation of particle size impact • Proper for fluidized bed gasifiers • Able to predict the product composition at different positions along a reactor	• Sensitive to the gas–solid contacting process • Computationally intensive • Limits their applicability to different plants

considerations render equilibrium modelling the more convenient method with which to study the general relations between fuel and process parameters and limiting syngas composition and yield. However, thermodynamic equilibrium may not be achieved in certain gasifiers and under many operating conditions, especially for gasifiers with relatively low operating temperatures [12,20,25]. Nevertheless, the models based on thermodynamic equilibrium have been the most widely used approach (see Fig. 2).

4.1.1. Stoichiometric vs non-stoichiometric models

The most widely cited subcategories of equilibrium models are stoichiometric (S) models and nonstoichiometric (NS) models. This review, and a complimentary more detailed theoretical analysis of the S vs NS method elsewhere [103], indicates that approximately 72.5% of equilibrium simulations in the literature to date use the NS method, and the remaining 27.5% use the S method.

However, as rigorously shown elsewhere [103], S and NS models yield identical predictions in virtually all practical biomass gasification scenarios. Hence, the other categorization introduced in this work, namely between Eq-single (Eq-sing) and Eq-separate (Eq-sep) models is more significant. The model choice between an Eq-sing or an Eq-sep typically does significantly change the yield and product composition predicted by the model. Given these facts perhaps too much attention has been given in previous reviews, and studies, to a model choice (S vs NS) that does not matter in terms of the model prediction (i.e. two different computational strategies to get the same result). The reader will find that a majority of the published equilibrium studies listed in this review do discuss, typically in their introduction, the motivation for choosing either the S or NS approach, but virtually none of these studies explicitly mention or motivate the consequential Eq-sing vs Eq-sep model choice they also did make.

In the stoichiometric case, the equilibrium of a preselected *set of reactions* are computed, while in the nonstoichiometric case, the equilibrium of a preselected set of chemical species are calculated. In both cases, thermodynamic property data—combined with either the assumption of ideality or a thermodynamic model (EOS + mixing rule or activity model) to account for non-ideality of the mixture—are used to compute the predicted equilibrium composition that will exit the gasifier.

The steps for the stoichiometric method are the following: 1) *Select the reactions* to be included in the simulation (in principle, the dominant reactions assumed sufficient to provide a useful estimate of the product gas compositions), 2) then calculate the equilibrium constants of these reactions at the reaction temperature, and 3), finally, compute the overall chemical equilibrium composition for a given feed composition (and pressure).

The explicit steps for the nonstoichiometric method are as follows: 1) *Select all the species* to be included in the simulation (in principle, all the chemical species that the modeler deems might be in the gasifier effluent in non-negligible amounts) and 2) then compute the resulting minimum Gibbs energy distribution among these chemical species for a given feed composition (which can be specified simply as the elemental composition of the feed [25,92]) at the reaction temperature and pressure.

The simplest implementation of both the stoichiometric and nonstoichiometric approaches is to compute only the gas-phase equilibrium. That is, in the simulation, one does not use the actual feed but rather an “effective feed” that consists of the actual feed minus the fuel (moles and mass of C) that will become a specified amount of ash and unreacted char. In this approach, the amount of ash in the char is an experimentally derived input parameter of the simulation. Essentially, the key question answered by both S and NS simulations (of the simplest gas only kind) is how all the gaseous carbon, oxygen, and hydrogen that ends up in the gas phase is distributed among the (gaseous) product species at ideal equilibrium at the temperature specified (or achieved in adiabatic simulation).

At this point, a key question is the following: Which of the two methods will better predict the composition of gasifiers that conform to assumptions 1 to 3 (listed at the outset of this section)? Or, alternatively, will the two methods always predict the same identical equilibrium composition? It is interesting that the literature is split down the middle on these questions. About half the gasification modelling studies published to date argue that the stoichiometric and nonstoichiometric approaches “are essentially equivalent” [20,103]. Conversely, about half the articles that address this topic indicate that the nonstoichiometric approach is more accurate [18,24,25,103,104]. Although not completely absent, the opinion that the stoichiometric method is more accurately predictive of reality is rare in gasification modelling (which is not necessarily the case for other reactive systems) [103]. So in summary, about half the researchers in the field predict that NS is better, and the rest predict NS and S is identical.

To clarify this situation, and the roughly even split in the literature as to whether these two approaches necessarily lead to identical results or not, we published [103] a mathematical proof that shows that for the gas phase equilibrium the exact solutions to the stoichiometric and nonstoichiometric models are identical. Hence, if a stable and consistent numerical algorithm is used the equilibrium predicted by both methods (S and NS) will be identical.

The choice between the stoichiometric or the nonstoichiometric method in modelling the basic gasification system is therefore purely a matter of expediency. These approaches are two different methods that converge to the exact some predicted composition. (The exception to this may be more complicated systems than those typically encountered in gasification modelling; systems where there is a subset of reactions that do approach equilibrium and a subset of reactions that do not and where this subset of non-equilibrium reactions limits the product yield.)

4.1.2. Eq-single vs eq-separate models

In addition to stoichiometric or nonstoichiometric, equilibrium models can be classified as Eq-sep (e.g. Refs. [31,36,37,49,62,63,72,83,90,91]) or Eq-sing (e.g. Refs. [6,11,17,33,34,40,44,46,48,54,61,70,71,89,105–107]) approaches. This classification is based on whether as in the Eq-sep case the char combustion is modeled as achieving a separate and distinct equilibrium independent of the reduction of the VM and un-combusted char, or alternatively (in the Eq-sing case) the combustion and reduction reactions achieve a single global equilibrium as one reactive chemical system. Our survey indicates that about 75% of published biomass equilibrium simulations are of the Eq-sing type, with the remaining 25% of equilibrium simulations being of the Eq-sep type (see Fig. 5). Schematics of the 'process flow' within the algorithms for each type is shown in Figs. 7 and 8 respectively. It can be seen that the Eq-sep approach assumes equilibrium only between the volatile components (produced in the pyrolysis step) and the char that is not combusted. Typically, either the fraction of tar combusted, or reduction zone temperature (which indirectly determines the amount of char that needs to be combusted to achieve the prescribed temperature) is a model input parameter. The Eq-sep approach thus models char combustion as occurring separately in a second heterogeneous reactor with heat flow from the second, exothermic 'combustion reactor' into the first gas-phase 'reactor' (even in single bed gasifiers where in reality there is only one 'reactor'). With the Eq-sing approach, the combustion and gasification of both the char and volatile gasses are modeled in a single reactor where a single overall heterogeneous equilibrium is assumed between all the components and all the reactions (combustion reactions and reduction reactions). Given that the choice between the stoichiometric and nonstoichiometric approach leads to identical solutions (see the discussion above [103]), but the Eq-sing and Eq-sep models typically will produce different final product compositions and yields, the choice between using an Eq-sing or Eq-sep model is more important. Yet notwithstanding this fact, this model choice is not discussed in any of the prior reviews on the modelling of gasification [18,20–25] while the discussion of the S vs NS enjoy wide discussion in the literature and introductions of simulation studies.

In the remainder of this section the modelling steps, differences and relative merits of the Eq-sing versus Eq-sep models will be discussed. For both models the first step is modelling pyrolysis. The pyrolysis step is an extremely complex part of the gasification cycle, having a large number of chemical and physical phenomena occurring rapidly and simultaneously. Generally, when dried biomass is heated in across a temperature range of 200–500 °C during the pyrolysis step, the biomass decomposes into solid char and volatiles (tar and gases) as shown in Fig. 6 [26]. For all model types the relative amounts of VM, char (also called fixed carbon) and ash (inert solid carbon) are typically computed based on empirically motivated input parameters. Within a stoichiometric model there needs to be a formula, or model, that determine not just the amount but also the molecular distribution of VM species produced by pyrolysis. The typical choice is to include H_2O, H_2, CO, CO_2, CH_4, N_2. Sometimes minor or trace elements like Cl_2, NH_3, H_2S and SO_2 etc. Is also included if modelling the fate of the relevant elements and species are of interest. When using a non-stoichiometric model, the VM needs to be specified only in terms of the *amount* of every element present. (If the Gibbs minimization equilibrium reactor is operated isothermally then the equilibrium product distribution does change if one changes the distribution of atoms among the species present in the input stream [103]). Hence, within the computational algorithms or flow chart of a non-stoichiometric model the volatile output from the pyrolysis step is typically expressed simply as equivalent amounts of C, H_2, O_2, N_2, Cl_2, and S that is fed to the Gibbs

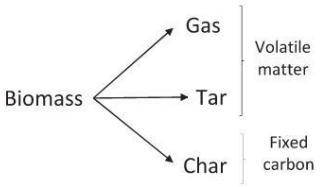

Fig. 6. Pyrolysis outputs.

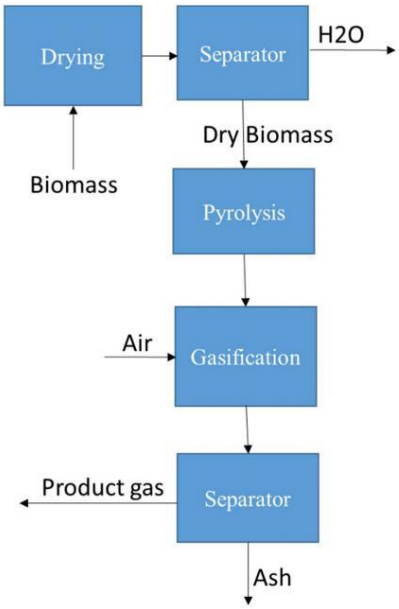

Fig. 7. Process flowchart of Eq-sing model.

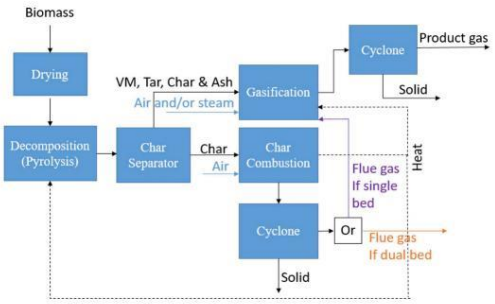

Fig. 8. Process flowchart of Eq-sep modelling.

minimization reactor. In both models char is also specified as a fraction of inert carbon produced in pyrolysis.

The pyrolysis outputs are not separated from each other in Eq-sing simulations. All three types of outputs in Fig. 6 enter the virtual gasifier (reactor in the model) together. The gasifier is a module that computes the global equilibrium of the gasification reactions based on the stoichiometric or nonstoichiometric approaches. A process flowchart of Eq-sing modelling is shown in Fig. 7.

In the Eq-sep model, char is typically subdivided into the fraction of char that will be combusted and the remainder. This fraction can either be specified or internally calculated if the gasifier temperature is specified (since the combustion of char provides and thus determines the temperature of the gasifier/equilibrium reactor). Hence the fraction of char to be combusted is separated from the volatile materials and sent to the a virtual "char combustion reactor" together with air. Char combustion produces heat that supports most of endothermic gasification reactions, as well as the energy required by the drying and pyrolysis parts (i.e. any of these models include heat transfer from the combustion reactor to the pyrolysis and gasification reactors or computation blocks). The residual solid char (char not fed to the combustion reactor) is fed together the VM, remaining air (if any is not fed to the combustion reactor) and steam (in application with additional steam agent) to the relevant equilibrium reactor modelling gasification step (combustion and reduction zone).

The gasifier equilibrium is computed based on the equilibrium constants (stoichiometric method) or minimization of Gibbs free energy (nonstoichiometric approach), and the combustor is modeled based on combustion equations (Table 1). The combustion is typically assumed to be complete. Alternatively, an empirically motivated amount of unreacted oxygen can be assumed, or a separate heterogeneous equilibrium can be assumed in the combustor. Finally, in most simulations, all unreacted char and ash is separated from gas components of the product stream(s) using a virtual cyclone(s).

As can be seen in Fig. 8 the Eq-sep model was likely developed to model dual bed gasifiers, where combustion indeed physically happens in a separate chamber than reduction. But, subsequent researchers also started using the Eq-sep approach for single bed gasifiers (by following the purple as opposed to the orange route for the flue gas in Fig. 8) where combustion and reduction happens in the same reactor albeit, for the most part in different zones (or areas) of the reactor. The potential benefits and motivation for using a strategy that physically corresponds more closely to a dual bed configuration also for a 'single bed' reactor will become clearer in the next few paragraphs.

The Eq-sing and Eq-sep models each have their own advantages and disadvantages. Eq-sing models are simpler in formulation however they frequently fail to yield satisfactory predictions of experimental gasification outputs. This failure is often attributed to the possibility that complete thermo-chemical equilibrium between all solid carbon (char atoms) and all gas-phase species may not be a realistic assumption for any given real-world gasifier. The notion of incomplete heterogeneous (solid-gas) equilibrium does explanation under prediction of equilibrium simulations of the amount of the residual char (or ash) produced in experiments. That is, for typical gasifiers, all gas-phase reactions and the gas-solid reactions most likely do not approach a single, perfectly global heterogeneous equilibrium where all solid phase atoms are accessible to all reactions. However, equally common deviations between equilibrium simulations (in particular ideal Eq-sing simulations) and experiments are the under prediction of the amount of CH_4 and/or CO_2 produced and an over prediction of the amount of CO and H_2 produced.

It is very common that all these deviations are compensated for by various quasi-empirical strategies. These include the pre-specification of amount of unreacted char (e.g. Ref. [108]), experimental adjustment or specification of some product components like methane (e.g. Refs. [75,109,110]), the use of an empirically adjusted (typically lower than actual measured) effective or quasi-equilibrium temperature rather than a single experimentally motivated lump average temperature (e.g. Refs. [111–113]) or empirical correction factors to the relevant equilibrium constants (e.g. Ref. [114]).

The Eq-sep method has the advantage that these empirically correlations and adjustments to ideal overall equilibrium can be more targeted and fine-tuned. Within the Eq-sep method the temperature of the combustion zone and reduction zone can be different, as in real gasifiers. Furthermore, heat flux between these can be adjusted to more accurately reflect imperfect heat transfer (which is real gasifiers is not instantaneous and infinite, i.e. there is losses and heat distribution to various gasifier zones is uniquely fractioned based on gasifier design and operating conditions). Note in Fig. 8 that it is important that the flue gas be sent along the right path that corresponds to the type of gasifier being modeled. In single bed gasifiers where the flue gas flow through the reduction zone the CO_2 (and/or H_2O) in the flue gas will shift or alter the WGS equilibrium (reaction R8 in Table 1) in the reduction zone. To not include this effect will be physically inappropriate.

In summary, for a dual bed or circulating gasifier the Eq-sep model is really the only viable approach. For a single bed gasifier, the Eq-sing model has less adjustable parameters and is simpler. (It gives a pure theoretical equilibrium limit of the yield obtainable in an ideal single chamber gasifier where all homogenous and heterogeneous reactions approach a single global equilibrium.) However, the adjustable parameters (fractioning of heat flow etc.) in the Eq-sep approach do correspond to realistic features of actual gasifiers. Additionally, while combustion typically safely can be assumed to go to completion, some reduction reactions, in particular methane reforming, do not tend to reach full equilibrium in many experimental tests. The Eq-sep model combined with the stoichiometric option provide the opportunity to exclude certain reactions from full equilibrium and model them separately, potentially in separate "virtual" reactors with heat exchange with other reactor blocks. This approach may, in some cases, more closely model real gasifiers where not all reactions operate close to equilibrium.

In summary, if the goal of an equilibrium simulation is to calculate purely the "thermodynamic limits", i.e. limiting yields obtainable under most ideal conditions – then the Eq-sing method achieves this goal with no assumptions or empirical fudge factors. However, if the goal of an equilibrium simulation is to predict the actual output of a non-ideal real gasifier, then the Eq-separate method provides more opportunities for targeted introduction of empirical adjustments and factors that correct just the specific aspects of the real gasifier (e.g. reactions or zones) that do not approach ideal equilibrium.

4.1.3. How accurate can equilibrium models be?

In general, equilibrium models predict only the physically possible limits in the performance of a given gasifier at the given operating conditions. The observed product composition and syngas frequently fall short of the equilibrium's ideal. The most commonly reported and noteworthy deviations between ideal equilibrium predictions and experimental observations are, first, higher amounts of methane in the final syngas (compared with the equilibrium methane concentration) and, second, larger amounts of unreacted char in some cases [23,108,115,116]. The unreacted char issue is best dealt with and avoided by only computing the equilibrium of the volatile gas-phase components rather than the complete heterogeneous equilibrium (Eq-gas approach) [90,92,103,112,115–117]. More accurate predictions can be obtained using empirical or experimental data (e.g., amount of residual char determined by experiments) to set the intimal conditions (atomic make-up and amount of volatile gasses generated). When it comes to higher methane yields than the equilibrium calculations predict, there is no easy work-around. It has been suggested that methane is released or formed during pyrolysis and that the methane gasification reaction rates simply are too slow in many gasifiers to fully approach equilibrium [23,108,116]. In such patently non-equilibrium conditions, in principle, only kinetic models could accurately predict the methane yields.

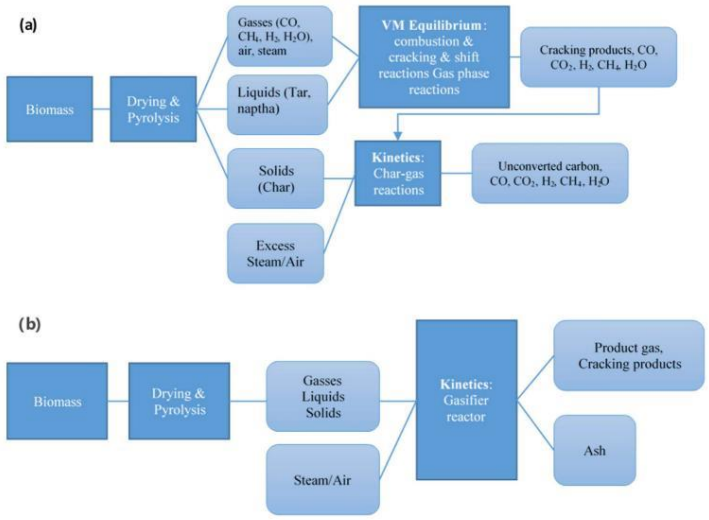

Fig. 9. Process flowcharts of (a) Kin-semi model, (b) Kin-total model.

How large can the deviations between the observed gasifier yield and composition and the relevant thermodynamic equilibrium predictions get for typical practical applications? Loha et al., for example, found that in a steam-fed fluidized bed gasifier, the deviation of the amount of actual methane produced grows larger rather than smaller at higher temperatures [118,119]. (This, of course, is exactly counter-intuitive and widely quoted general rule of thumb that higher temperatures should be necessarily close rather than increase the gap between the equilibrium and measured composition.) For example, at 750 °C and a steam-to-biomass ratio of 0.6, the total percent of syngas composition measured to be methane by Loha et al. was 4.2 vol% compared with an equilibrium methane fraction that would be only approximately 2 vol% [118]. Cases like this where the observed amount of methane is double, or even just more than the equilibrium amount, are fairly common [118–120]. Deviations between the equilibrium amounts and experimentally measured amounts of other syngas components (H_2, CO, CO_2) are invariably much less drastic (within 5 vol%) than the methane deviations that can occur in certain gasifiers [118–121].

4.2. Kinetic models

To precisely predict the non-equilibrium product distributions, kinetic modelling is required. Kinetic models can also predict gas composition and temperature profiles throughout the various gasifier zones as well as the evolution of these variables in time during non-steady-state operations and start-up. Because kinetic models have spatial resolution, they by necessity require detailed fluid dynamic modelling in addition to the kinetic model. In general, kinetic modelling can include not only the reaction kinetics and transport but could also include a model of the particle size distribution (and its evolution through the gasifier), micro-scale mass transport (e.g. diffusion into char particles) and mixing inside the gasifier. Notwithstanding this complexity that is potentially necessary to capture all the consequential physics.

Kinetic models can be very accurate and detailed, but this accuracy is difficult to achieve in practice since these models attempt to describe very complex phenomena, such as gas-solid-particulate fluid flows, gas–solid contacting process and microscopic evolution of particle distributions, which is hard to model reliably. There is however significant ongoing work aimed at developing the detailed kinetic and CFD models and rate laws required to accurately describe the reaction rates and transport of gasification. This work, by individual contributors or groups like for example the CRECK consortium or Reacting Gas Dynamics Laboratory [122,123], span ab initio methods and experimental approaches [123–136]. However, in the case of fluidized bed gasifiers complex solid–fluid contact patterns result in large deviations from ideal equilibrium compositions (and ideal mixing), and hence for fluidized bed gasifiers the detailed kinetics need to be combined with realistic hydrodynamic modelling; kinetic-hydrodynamic modelling therefore is a particularly common and necessary approach chosen for modelling fluidized bed gasifiers, as argued by several authors [26,29,38,39,43,52,55,57,65]. The promise of potentially more accurate results motivates about 34% of the researchers who model gasification to employ simulations that model the kinetics of key reactions (see Fig. 5). As suggested, kinetic models can be divided into Kin-semi (e.g. Refs. [26,38,57]), Kin-total (e.g. Refs. [28,29,39,53,65,73,74,82,84,86]), and Ki/Eq (CRF) (e.g. Refs. [32,41–43,59,137]) approaches. Among articles with kinetic rate expressions in them our survey found that roughly 48% of biomass gasification studies published from 2000 to 2017 used a Kin-total model, roughly 24% used a Kin-semi model, and the remaining 28% used reversible rate expressions that limit to the thermodynamic equilibrium and empirical correction factors for the heterogeneous char reactions (the so-called CRF method).

The Kin-semi approach assumes local equilibrium for some reactions and/or gasifier zones but computes kinetically controlled concentrations and temperatures for other zones and/or reactions. Unlike the equilibrium models considered in section 4.1 the Kin-semi approach separates char from volatile matter (see Fig. 9A). Char—the product of the drying and devolatilization step, is often modeled using the approximation that it consists of carbon only [28]. Like pyrolysis, char gasification is a complex process. It involves mass transfer (adsorption, diffusion, desorption, etc.), multiple chemical reactions, multiphase heat transfer, and so forth. The main chemical reactions of char gasification can be classified and subdivided into homogeneous and heterogeneous reactions (Table 1). Although there can be several

variations in the way equilibrium and kinetic calculations are combined, the most common implementation is the one shown in Fig. 9A (examples are [26,52,55,60,138]). In this, the most typical type of Kin-semi model, the volatile matter generated in the pyrolysis step first enters a volatile reactions module where a homogenous gas-phase equilibrium is computed by equilibrium constants or the minimization of Gibbs free energy. This equilibrated gas mixture is then fed, together with air/oxygen and/or steam and the solid char, into a kinetic module (which can be CSTR or a PFR) where reaction rate kinetics are used to determine the final composition from the reduction zone and where char gasification occurs. (Typical recent examples are [26,139]. For alternative Kin-semi variations see, e.g. Ref. [57]).

Within Kin-total models, reaction rate kinetics simultaneously model both the volatile and char gasification reaction rates and local temperature and composition as the simulation code step through the reactor (which can be of any type, with the CSTR or PFR being the most common). Kin-semi models require less kinetic rate laws and parameters than Kin-total models. As a result, Kin-semi models can be more accurate than Kin-total models if the reactor conditions are such that the gas phase is close to the chemical equilibrium. Conversely, Kin-total models with reliable rate laws and hydrodynamic models are, in principle, the only option that could accurately describe non-ideal reactors and operating conditions.

4.3. Kinetic/equilibrium (CRF)

To complete this survey of modelling approaches one further modelling approach or category is proposed for a type of model (Ki-CRF) that does not fit neatly into either of the equilibrium categories or kinetic model categories considered this far. Unlike the Kin-semi method, the Ki-CRF approach models the reduction zone kinetically (i.e., all reactions and species concentrations are computed with a PFR-style rate law-based reactor model). However, the rate equations used in the reduction are typically formulated as a relatively simple Arrhenius type reversible reaction that includes the equilibrium constants in the rate expressions to make all the equations thermodynamically consistent. Additionally, the pre-factors of these rate expressions for the reactions involving char are typically empirically adjusted by multiplying them with an adjustable parameter called the char reactivity factor (CRF). As such, this approach is a true hybrid of kinetic reactor modelling, thermodynamic equilibrium data, and empirical adjustments.

Ki-CRF models are designed to model gasifiers where the chemical composition of the product gas is not equal to the equilibrium composition, as is, for example, common with fluidized bed gasifiers. Ki-CRF models furthermore acknowledge the reality that truly reliable rate laws for especially heterogeneous char gasification reactions may not be available and that it may be more expeditious to utilize general thermodynamic equilibrium data and empirical CRFs in relatively simple rate expressions.

Generally, pyrolysis and cracking reactions are not considered in these models because the number of possible pyrolysis products with all the possible reactions and intermediate products would make the model very complex. Moreover, Ki-CRF models start at the top of the reduction zone, so all the gasification calculations would be based on an empirical estimate of the initial feed into this section (assumption and empirically motivated estimates of the extent of combustion and pyrolysis). Hence, the accuracy of the model is limited by the availability of data on the initial conditions at the top of the reduction zone.

4.4. A survey of the models in the literature

A representative survey of studies modelling gasification is shown in Table A. 1 (in Appendix A Supplementary materials) [11,17,26,28,29,31–44,46,48–50,52–54,56–58,61–63,65,67,68,70–74,82–84,86,89–91,105,106,137,140,141]. The table can be consulted to quickly identify works relevant to certain types of gasifiers, feedstock, agents, and operating regimes or, conversely, to see how widely a given modelling approach has been applied across these applications (or not). It is clear from Table A. 1 that the number of variables both in terms of the physical variations modeled (gasifier type, agent choice, and feedstock) and the modelling approaches used (Ki or Eq) are large enough that many combinations have been studied, yet some others have not. This section will discuss some conclusions drawn from the survey data regarding what application areas have been well studied in the literature and what gaps or under studied areas may exist.

The data indicate that roughly more than 50% of the published works to date model fixed-bed gasifiers of mostly the downdraft type (downdraft gasifiers make up around 85% of the cases simulated in these fixed-bed studies, that is, fixed-bed downdraft gasifiers currently are the most popular gasifier to simulate, representing roughly 42.5% of all published simulation studies). Furthermore, our survey shows that most of the downdraft modelling utilizes thermodynamic equilibrium calculations, with more than half of all downdraft studies (~55%) using the Eq-sing approach. Moreover, it can be seen that the simulated operating temperature, steam to biomass ratio, air to biomass ratio, and equivalence ratio for downdraft gasifiers are in the ranges of 673–1673 K, 0.05–0.55, 1.35–1.9, and 0.1–0.9, respectively.

In addition, more than 80% of the downdraft models were used to simulate one or more species of untreated or pure wood (most typically in wood chip form) with air and steam as the gasification medium. In our survey, just Barman et al. [33] developed a model to simulate the gasification of treated wood with a downdraft gasifier. Barman et al.'s [33] model is designed to simulate a fixed-bed downdraft gasifier. It is proposed that tar formation can be more significant when gasifying treated wood compared with clean wood. Barman et al. [33], however, also argued that the complexity of tar formation prohibits the predictive modelling of tar; hence, they instead simply used experimentally reported tar yields as fixed a priori *input* parameters in their simulation work (i.e., the simulations predict just the final distribution/yield of H_2, CO, CO_2, CH_4, and H_2O). Barman et al. [33] reported that their model predictions show fairly good agreement with results from prior models and various experimental investigations published by others. Following this validation, they used their model to predict the optimum operating gasification temperature for straw, treated wood, and untreated wood.

Table A. 1 shows that around 40% of the published models are designed to model fluidized bed gasifiers. Circulating, bubbling, and entrained gasifiers all are represented in the models, with the most common subclass of kinetic model used being the Kin-semi approach. Moreover, the data show that when it comes to fluidized bed gasifiers, the following ranges of operating parameters have been of interest and hence have been simulated to date: temperatures of 600–1600 K, steam-to-biomass ratio (S/B) of 0–5, air to biomass ratio (A/B) of 1.25–5, and equivalence ratios (ER) of 0.29–0.38.

Finally, terms and conditions of employing different modelling approaches are shown in Table 3. As it shown, Equilibrium modelling methods can only be used to predict reliably fixed-bed gasifier performance as a function of feedstock and given information about operational conditions. Kinetic modelling approaches can also present good approximation for fluidized-bed gasifiers at low temperature. Ki-CRF models can be also applied when reliable rate laws for especially heterogeneous char gasification reactions are not available and that it may be more expeditious to utilize general thermodynamic equilibrium data and empirical CRFs in relatively simple rate expressions.

4.5. Tar modelling

It is worth considering the thoughts of alternative fuel and biomass gasification pioneer Thomas Reed [99], as follows:

"While a great deal of time and money has been spent on biomass gasification in the last two decades, there are very few truly commercial gasifiers, operating without government support or subsidies, day in,

Table 3
Terms and conditions of using different modelling approaches.

Modelling approaches	Terms of use
Eq-single	• Using Fixed-bed gasifier • Feedstock with low Tar content • High operating temperature (750–1000 °C) • Lack of information about chemical reactions
Eq-separate	• Using Fixed-bed gasifier • Feedstock with low Tar content • High operating temperature (750–1000 °C) • Existence of information about chemical reactions
Kin-semi	• Using Fluidized-bed gasifier • Low to medium operating temperature • Lack of data about reactions kinetics and hydrodynamics for combustion, cracking, shift reactions and gas reactions
Kin-total	• Using Fluidized-bed gasifier • Low to medium operating temperature • Existence of data about reactions kinetics and hydrodynamics trough all parts of gasifier
Kinetic/Equilibrium (CRF)	• Using Fluidized-bed gasifier • Unavailability of truly reliable rate laws for especially heterogeneous char gasification reactions • Existence of empirical estimate of the initial feed into the gasifier

day out, generating useful gas from biomass. The typical project starts with new ideas, announcements at meetings, construction of the new gasifier. Then it is found that the gas contains 0.1–10% 'tars.' The rest of the time and money is spent trying to solve this problem. Most of the gasifier projects then quietly disappear. In some cases the cost of cleaning up the experimental site exceeds the cost of the project! Thus 'tars' can be considered the Achilles heel of biomass gasification. In the gasification of coal, a more mature technology, the 'tars' (benzene, toluene, xylene, coal tar) are useful fuels and chemicals. The oxygenated 'tars' from biomass have only minor use. With current environmental and health concerns, we can no longer afford to relegate 'tars' to the nearest dump or stream."

Indeed, tar may be the single most important impediment to the practical implementation of biomass and organic waste gasification [7,10,99,125,142] and a significant factor in environmental pollution from gasification [143,144]. Tar has not only been neglected relative to other performance metrics in research studies, but perhaps also in the simulation sphere. All the articles included (see section 2) in our representative review suggest that just under 12% of all biomass gasification studies published from 2000 to 2017 include any tar modelling whatsoever. This section provides a brief overview of tar modelling approaches published to date.

The products of biomass gasification are of three types: gases, condensable tars, and solids (char and ash). By definition, tars are any condensable (mostly organic) compounds in the gasifier product stream [99]. Tar is generated predominantly during pyrolysis [98]. The subsequent fate of pyrolysis tar is then either to be cracked and gasified (reduced), combusted or it may persist (including transformation or "maturing" to higher molecular weight PAHs or soot) through combustion and reduction zones, in which case the residual tar either exists with the product gas or condenses and is deposited on downstream components [98,99,144]. The "stickiness" of tar condensate makes managing tar in downstream equipment an important practical challenge. For all these reasons, the modelling of tar formation and persistence in high tar-producing applications such as biomass, municipal waste, or plastic gasification is of growing interest [10,21,26,28,123,141,145]. However, the precise chemical composition of tar can be complex—Milne's lists of components contains 69 primary, 87 secondary, and 36 tertiary species, with the caveat that this list is partial and that "literally hundreds of other compounds have been identified in pyrolysis" [99]. Given that tar consists of a complex mixture that varies greatly depending on the process' operating conditions, feed, and gasifier type [21,99,123], it should be no surprise that the precise chemical description of tar in all models invariably is and needs to be simplified, one with no simple and preferred one-size-fits-all formula [21]. Table A. 2 (in Appendix A Supplementary materials) provides an overview of the tar modelling choices made to date.

From Table A. 2, the chemical representation of tar currently is done with very simple models consisting frequently of only one—and at the most four—representative model compound. The estimation of tar yield is a difficult task using a thermodynamic equilibrium model because tar is typically a non-equilibrium product. Therefore, the predictions of tar yield in equilibrium models are mostly empirically fixed independently of the gasifier operating conditions, in accordance with other literature models. Moreover, in equilibrium models, tar is set as an inert component in the gasifier reactor; hence, tar cracking and tar reduction models are not possible. However, in kinetics models, tar decomposition has been mainly modeled because of cracking and steam and dry reforming reactions, as shown in Table A. 2.

5. Conclusion

A new classification of the most important gasification modelling approaches was presented, and the representative statistics of the frequency of their use was collected. Although the most appropriate choice of model depends on factors such as the goals of the simulation, the type of gasifier, feedstock, and operational parameters several general observations can be made.

For modelling downdraft gasification in particular, equilibrium models are typically a good starting point. Downdraft gasifiers frequently operate not too far from equilibrium because of their relatively simple geometry (and hence simpler hydrodynamics) and because of the relatively high operating temperature they typically employ. Furthermore, in downdraft gasifiers, both pyrolysis and gasification products are forced through the oxidation zone so that equilibrium is obtained after a brief time period [20]. It also can be observed from Table A. 1 that more than 65% of downdraft models employ the Eq-sing approach. Eq-sep models introduce somewhat more complexity and abstraction in formulation, but their predictions can be more accurate compared with Eq-sing models, as shown by the studies surveyed here. Moreover, Eq-sep models allow the researcher to assess in greater detail the impact of additional design features, such as the degree and location of combustion, heat transfer and loss from and between gasifier zones, and the effect of heat recovery from flue gas.

Even for the research that does embark on the more complex task of formulating a kinetic model, it still may be advisable to also run an equilibrium model of the same application. In gasification, equilibrium can play the same role as in any other chemical system, namely revealing the thermodynamic limits of operation and how these limits depend on operating parameters and inputs (e.g., heat recovery, equivalence ratio, biomass moisture content, and steam injection). A drawback in using equilibrium modelling only is its inability to evaluate the impact of hydrodynamic parameters on gasification. If the goal is to optimize or understand the effect of parameters such as particle size distributions, feed density, and reactivity on the outlet gas composition, carbon conversion, and system performance, then a kinetic model would be required. However, the kinetic models generally contain kinetic and transport parameters that are hard to come by. Even if these parameters are measured, the resulting model will to some degree be limited to the specific gasifier type and design, feedstock, agent, and operating range combination for which the rate expression form and parameter values are valid.

In section 4.5 approximation methods used for tar modelling were surveyed. Tar modelling is likely to become one of the most active areas of research because of the central importance of tar avoidance for developing practically feasible and environmentally responsible biomass and waste (including plastics) gasification technology. Developing

modelling approaches that can adequately provide scientific insight and/or practical operator guidance on how to manage tar formation is perhaps the most urgent challenge to be taken up by the biomass gasification modelling community.

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Appendix A. Supplementary data

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Paper III

The equivalence of stoichiometric and non-stoichiometric methods for modeling gasification and other reaction equilibria.
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The equivalence of stoichiometric and non-stoichiometric methods for modeling gasification and other reaction equilibria

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ABSTRACT

The chemical equilibrium of gasification systems is modeled using one of two approaches, the stoichiometric (S) or the non-stoichiometric (NS) method. A complete survey of the gasification literature shows that about half of equilibrium modeling studies use either just the S, or just the NS method, and do not consider whether a different model choice would lead to a different solution. The remaining half of equilibrium modeling studies does motivate their model choice. Among those that discuss their model choice roughly half (15/27) state that the two approaches produce identical solutions. The remaining half propose that the NS method yields superior results (10/27), or the S method may yield superior results (2/27), and thus imply that the methods are not necessarily equivalent. The contradictory conjectures on both sides are made without definitive proof, or reference to definitive proof or evidence. In addition to providing a concise technical review of this question and its role in biomass gasification modeling, a second goal of this technical review article is to provide a tractable, yet rigorous and definitive exposition of the mathematical proof that the stoichiometric and non-stoichiometric approaches are equivalent methods for computing the equilibrium composition of the core gasification problem. This should provide perspective on the existing literature, and helpful guidance for future modeling work. Although the technical review and analysis provided here settles a longstanding contradiction in the gasification literature the relevant proof applies to any reactive system. The systematic template for S vs NS equivalence provided here should therefore be equally useful to researchers modeling and simulating the equilibrium of any other reactive system, since there is always the need to choose between the S or NS approach.

1. Introduction

The aim of this technical review is two-fold:

1. Summarize the assumptions and claims in the literature regarding the equivalence of the stoichiometric (S) or non-stoichiometric (NS) approach for modeling gasification.
2. Resolve the existing contradictions in the literature by providing the rigorous mathematical criteria for when the S and NS models will yield identical solutions, and when not.

We can summarize the conclusions at the outset:

1. The review will show that approximately half of all authors that published equilibrium models for gasification chose either the S or NS approach and did not not motivate or discuss the choice [1–22]. The remaining half is roughly split 50-50 in the following way: Approximately ¼ of published gasification equilibrium studies chose either the S or NS approach and motivated their choice by claiming the method they chose will yield superior (closer to experimentally observed) results. The remaining ¼ of authors suggest that the S and NS approaches will yield "similar" [23,24] or "identical" [25–38] results and they therefore chose one or the other approach based on numerical expediency or simple preference.
2. We could find no author that either provides a proof, or reference a source with the relevant mathematics, that rigorously settle this roughly 50-50 disagreement in the literature on whether the S and NS models predict the same equilibrium, or different equilibria, for the gasification problem. We therefore provide the relevant mathematics that settles this question here as part of this technical review and in the appendices (supplementary material). For the basic formulation (see definition below) of the gasification problem the S and NS models are equivalent and do yield identical solutions. Many studies use more complex models than just the basic formulation. For the most part equivalence will be retained for more complex systems,

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Nomenclature

A_S	set of all rearrangements of all atoms in the system into the molecular species present as reactants or products in *the reactions specified*
A_{NS}	set of all possible rearrangements of all atoms in the system into the molecular species specified
$K_{eq,j}$	equilibrium constant for reaction number j
NS	non-stoichiometric method
S	stoichiometric method
SMR	steam methane reforming reaction
T	temperature °C
WGS	water gas shift reaction
m	number of chemical species (molecules) specified
n	number of distinct elements (atom types)
r	number of independent chemical reactions specified
r^*	Critical value of r at which the S and NS methods become equivalent
n_i	number of moles of species i mole/s
n_{i0}	number of moles of species i in feed or initial condition mole/s

Greek Letters

ξ_j	extent of reaction (of reaction j) mole/s
ν_{ij}	stoichiometric coefficient (for molecular species i in reaction j)

SubscriptsRange

i	label for molecular species 1, 2, …, m
j	label for chemical reaction 1, 2, …, r
k	label for atom type 1, 2, …, n

Symbols

$\subset$	proper subset
$\subseteq$	subset
$\equiv$	equivalent (identical) set
$\bar{}$	vector
$=$	matrix

Operators

col(A)	number of columns of matrix A
null(A)	dimension of the nullspace of matrix A (nullity)
rank(A)	number of linear independent columns of matrix A
row(A)	number of rows of matrix A

but equivalence is not universally guaranteed. Equivalence cannot be assumed; it should be checked. We provide the rigorous mathematical check, or procedure, that any researcher or author can follow to verify whether for their system the S and NS methods will yield identical solutions, or could potentially yield different solutions. (system = choice of modeled molecular species, modeled phases and for the S formulation also the set of reactions included.)

General introduction. Biomass and energy from waste is currently the largest non-fossil fuel source of energy utilized by humankind [39]. Gasification is one of the most economical and flexible among the methods used to extract energy from biomass and organic waste. The flexibility includes the type of feedstock (inputs) and the form(s) of energy produced (outputs) [40–42].

An important aspect of gasification research is modeling and the majority of these models are equilibrium models [39]. The number of published studies modeling the chemical equilibrium composition of various gasification scenarios and applications is growing steadily [23,24,39]. In a recent comprehensive review we reported that approximately 60% of all published gasification studies with models used only equilibrium models and just 40% used, or included, non-equilibrium deviations based on kinetic and transport/CFD models [39]. Moreover, the fraction of 'equilibrium only' studies appears to be growing since 2000. For example, roughly 50% of published models in 2006–2009 were 'equilibrium only' compared to roughly 75% of models in 2014–2017 being 'equilibrium only' [39].

In many studies the predicted equilibrium compares reasonably well with the product distribution observed in experiments [39,43,44]. In other cases the deviation from equilibrium is small enough so that the experimental composition can be systematically correlated to the equilibrium composition [9,28,42,45–47]. Even when the product stream from a gasification system does not approach the equilibrium composition, knowledge of the chemical equilibrium still is desirable since the equilibrium sets the achievable limits of operation and thus the potential room for improvement that could be achieved with the optimization of the gasifier design and/or the operating parameters. Any engineer worth her or his salt would want to know is there potential room for improvement or not. Equilibrium models are and will remain relevant.

In all gasification modeling and design work it is vital that researchers know that they compute the appropriate chemical equilibrium correctly and accurately. There are two approaches that can be used to model and predict the equilibrium composition for any system of chemical reactions in general, and the gasification equilibrium in particular. The two approaches are typically designated as the stoichiometric (S) or non-stoichiometric (NS) methods [42]. When implementing the S method a set of r independent chemical reactions are specified, thereafter the initial concentrations of all chemical species are specified. The equilibrium concentrations are then calculated by solving for the extent (ξ_j) of every reaction j (utilizing the relevant equilibrium constant $K_{eq,j}(T)$ and the standard equilibrium expression of chemical thermodynamics, together with a molecular mole balance for every chemical species). Readers will undoubtedly recognize the S method as the methodology taught universally in undergraduate chemistry courses where the S method is colloquially referred to as 'computing the chemical equilibrium with equilibrium constants' [48,49].

When implementing the NS method, no reactions are specified, instead the researcher only specifies all possible reactant and product chemical species (molecules) that the researcher predicts, or knows (e.g. from experiment), to be present in the system. When implementing the NS method the initial concentrations of all chemical species merely specify how many moles of every element (how many atoms of every type) is in the system. The atoms are then distributed between the possible chemical species (reactants and products) in all possible combinations and the distribution that minimizes the overall Gibbs energy of the system is computed. In summary, the S method requires the specification of a set of r independent chemical reactions (involving m chemical species) that will be solved for their collective reaction equilibrium. With the NS method a set of m chemical species is specified and the method in principle consider all possible distributions of the atoms in the system between these m chemical species to find the distribution that minimizes the Gibbs energy of the system.

At this point the reader, familiar with the theory of chemical thermodynamics, and the derivation of the standard reaction equilibrium expression, will no doubt recall that the S method solution also "minimizes the Gibbs energy" [48–50]. Hence solutions obtained by the S method, and the NS method, both "minimize the Gibbs energy of the system" in some sense.

Are these solutions, namely the equilibria predicted by the S vs the NS method necessarily the same?

The mathematics in section 3, and counter examples provided in appendix 2, proves that *in general the answer is no*. The S and NS methods are not necessarily and always equivalent for any chemically reactive

systems. The can predict different equilibrium compositions.

However, for many problems or systems the S and NS methods can be shown to be mathematically equivalent. The most basic gasification problem is such a system. *For the basic gasification equilibrium as defined rigorously in section 3, the S and NS methods will always yield identical solutions*. (Assuming of course consistent and stable numerical algorithms are used that is fully converged to the unique identical solution – that is assuming no numerical programing or approximation error.)

In summary, the chief motivation for this review article is to point out, and then resolve, a misconception implied by much of the gasification literature that solutions obtained by the S method (reaction equilibrium approach), and the NS method (Gibbs minimization approach), are *necessarily* and *always* the same. This is not true in general. This is however true for the most typical and most basic formulation of the gasification problem (as will be rigorously proven here). Finally, we will also review a second significant portion of the gasification literature that make the opposite mistake, namely articles that state or imply that the S vs NS methods will yield different results for the gasification equilibrium. A belief that can be shown to be mathematically false for the baseline gasification equilibrium problem.

The flow of the rest of this article is as follows:

Section 2. A review S and NS model equivalence in the gasification literature.

Section 3.1 The S and NS model can in general be non-equivalent/predict different equilibria.

Section 3.2 Mathematical steps to check whether S and NS methods are equivalent and equivalence proof for the basic gasification problem.

Sections 3.3 Discussion of a few misconceptions in the literature.

Section 4 Conclusions.

Note: For the sake of clarity we will only discuss the isothermal

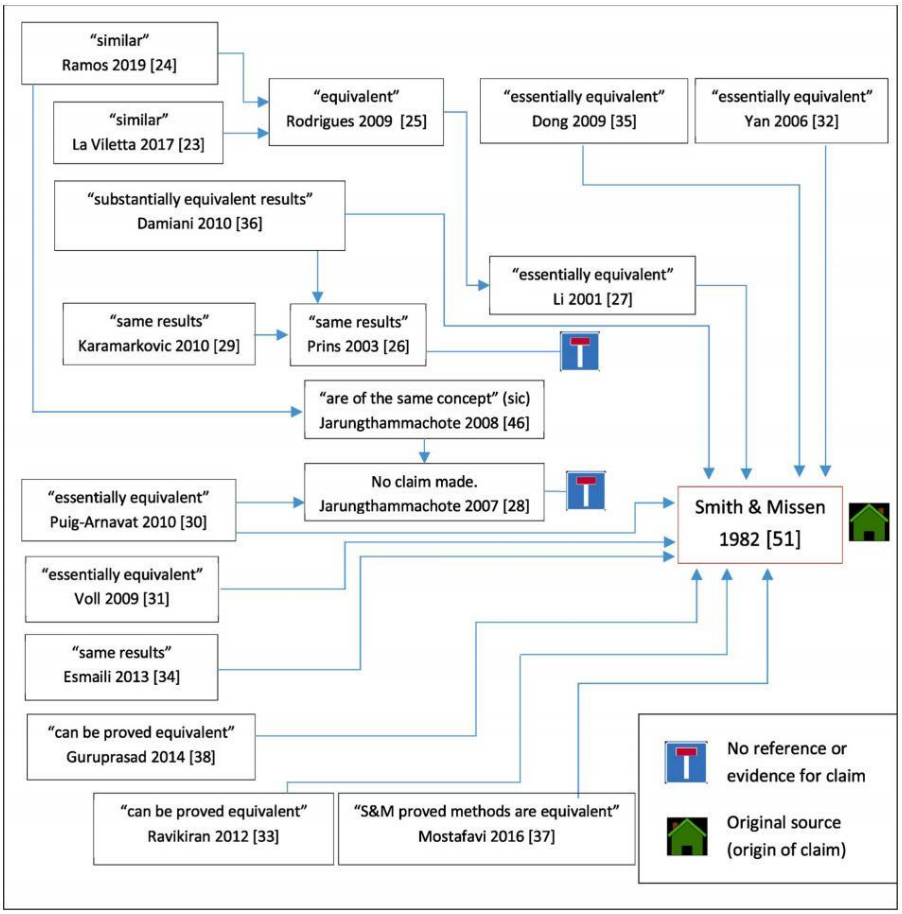

Fig. 1. A citation map for all references in the gasification literature claiming that the S and NS methods are "equivalent" or to some degree interchangeable. The exact phrase form every publication used to denote the "equivalence" is also provided since it succinctly suggests the nature of the equivalence assumed (ranging from similar to rigorously identical). All references map back to Smith & Misen 1982. The two exceptions are Prins 2013 that claims the S and NS methods produce "similar results" without any motivation or reference. Jarungthammachote 2007 makes no claims regarding equivalence. Smith & Missen 1982 does not have a proof of the type implied by the other references, the 'equivalence' proved in Smith & Missen 1982 has different more limited meaning (see text below).

reaction equilibrium problem in this article. All the ideas and proofs presented can be generalized to the adiabatic problem by adding an energy balance.

2. Technical background

2.1. Literature review and analysis

Fig. 1 is a comprehensive citation map that tracks all these references. It is clear upon examination of this map that all the references in the gasification modeling work reviewed essentially duplicate or copy each other, and that they all point back to a single publication or single primary source - namely a 1982 book by Smith & Missen [51]. This book, titled "Chemical reaction equilibrium analysis: Theory and algorithms" is an early compendium of numerical techniques from the era when personal computers became common place and numerical simulation became widespread. This book does not contain any proof that can be used to establish S vs NS equivalence (see Appendix 1 for a detailed discussion). There are however classic theorems in linear algebra that can be used to establish, or disprove, S vs NS equivalence in any given case. We will discuss these foundational mathematical theorems, and their application to the contradiction and confusion in the gasification modeling literature, in section 3 below.

Hence, the first group of authors in the literature state correctly (as we will establish rigorously below) that the S vs NS method will yield the same result, namely the same equilibrium prediction for the gasification problem as it is most typically formulated. For these authors the choice they made between the S and NS approach is typically described as merely a matter of personal preference or computational expedience.

In contradiction to the authors that suggest 'equivalence', there is a second roughly equally large group of authors in the literature that suggest or claim firstly that the methods are not equivalent, and secondly subsequently most typically claim that the NS method provide superior (more experimentally relevant or accurate) results [44,45,52–60]. We also found two outliers among group two (those who suggest that the S and NS methods are not equivalent) suggesting that the S method does produce [61], or could produce [62], superior results for their gasification applications. (Hence, we observe that among those implying non-equivalence of the two methods the overwhelming majority suggest that the NS method is more physically relevant. Claims of the S method performing better than the NS method seem relatively rare in gasification, but in some other non-gasification reactive systems the support for NS superiority can be less unanimous, e.g. Ref. [63,64].)

Correcting this contradiction (between the contradictory claims by the two roughly equally large camps or sides in the gasification modeling literature) and providing substantive references pointing to the relevant mathematical arguments is the primary motivation of this technical review.

2.2. Minimization of gibbs energy with concise set theory notation

As suggested in section 1 both the S and NS methods minimize the Gibbs energy in some sense as is illustrated in Fig. 2. However, it is immediately obvious from the illustration in Fig. 2 that the S and NS methods need not necessarily find the same minimum. For some S problem formulations, the number of independent reactions r cannot access all possible atomic re-arrangements. In this case the global NS problem Gibbs minimum may, or may not, differ from the S problem minimum. Hence for some values of r below a critical value r^* "equivalence" is not given. In section 3 we will formulate the rigorous mathematical criterion and procedure for calculating the critical maximum value r^*, such that if $r = r^*$ then the S and NS method equivalence is rigorously established and the two methods will necessarily and always have identical solutions. (We exclude the possibility $r > r^*$ because r is by definition the independent reactions, and it can be shown that if $r > r^*$ then the set of r reactions are not algebraically independent.)

Hence, the two approaches may, or may not, provide the same answer, and that S vs NS equivalence or non-equivalence depends on whether the global minimum Gibbs energy over all atomic redistributions (NS minimum) is included within the subset of atomic redistributions sampled by the S problem under consideration.

In order to provide a precise and concise proof, we will state our problem in the notation of set theory. Let A_S denote the set of all possible combinations (chemical compositions) $\{n_1, n_2, \cdots, n_m\}$ that are possible rearrangements of the a different types of atoms in the system possible by the r independent reactions specified in the problem statement. Recall that allowable (physically attainable) extents $\{\xi_1, \xi_2, \cdots, \xi_r\}$ is defined as any set of ξ_j for which all $n_i = n_{i0} + \sum_j^r \nu_{ij}\xi_j \geq 0$ for all m molecular species i. This is called the non-negativity conditions or constrants. (For

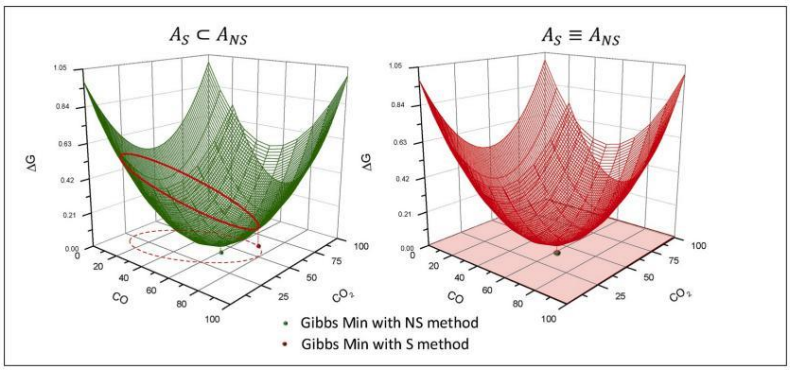

Fig. 2. Illustration of two cases. On the left the set A_S (corresponding to the dashed red line) of all atomic rearrangements (possible by r possible reactions specified) of the atoms present initially in the system is a proper subset of all possible rearrangements (when any rearrangement or conceivable non-nuclear reaction is possible). In this case the equilibrium (minimum Gibbs value subject to the constraints) could be substantially different for the S vs the NS problems. On the right is shown the case where the r reactions specified can rearrange the atoms in the system into all possible molecular re-arrangements, *i.e.* we have $A_S \equiv A_{NS}$ (area shaded red). In this case the S and NS methods will have identical solutions. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

example, the initial condition $\{n_{10}, n_{20}, \cdots, n_{m0}\}$ would be a trivial member of A_S , namely the member obtained by setting the extents $\xi_1 = \xi_2 = \cdots \xi_r = 0$ for all r reactions.) Let A_{NS} denote the set of all possible compositions $\{n_1, n_2, \cdots, n_m\}$ that are *any rearrangements or redistribution* of the a different types of atoms in our system into the m molecular species. Clearly we always have $A_S \subseteq A_{NS}$.

There are in general two possible situations. For a given application we could have $A_S \subset A_{NS}$. In this case, namely the proper subset case, the Gibbs minimum subject to the S constraint could be higher than the universal Gibbs minimum obtainable over the larger set A_{NS} (see Fig. 2). The second alternative case is $A_S \equiv A_{NS}$. If this case holds in a given application, then the Gibbs minima of the S and NS constraints become identical. In the latter case the solutions of the S and NS methods both are the minimum of the exact same objective function over the exact same space. We will provide examples of realistic chemical reaction systems of both kinds. For some chemical systems S vs NS equivalence is a reality. (For these systems the two methods always give identical solutions.) For other chemical systems it is not. (For these systems the two methods can and sometimes do give different solutions, i.e. the two methods predict different equilibrium compositions.)

3. Results

3.1. Examples of the type $A_S \subset A_{NS}$ (chemical systems where the S and NS methods are not equivalent)

A superficial reading of the fact that both the S and NS approaches 'minimize the Gibbs energy of the system', and/or a misinterpretation of a proof given by Smith & Missen 1982 [51] (see Appendix 1), may have led to a common notion in the gasification literature that the S and NS methods *always* predict the same equilibrium product distribution. It is important that we start by definitively disproving this notion of universal equivalence. The S and NS methods are not *always* equivalent. They can be for a given problem formulation, but one needs to establish that fact anew for every new problem or problem formulation. We will systematically go through the proof for the gasification problem in section 3.2. Here in section 3.1 we will motivate that the check is necessary.

Smith & Missen themselves were aware of the fact that in many chemical systems all possible reactions do not occur, and that this latter fact in some cases does introduce additional constraints to the chemical equilibrium observed in real world experiments [65]. That is, in some applications the S method solution with a judicious selection of reactions, may be both different than, and more physically relevant than, the "more stable" equilibrium predicted by the NS method. As our first example of such a system we choose an example furnished by Smith & Missen themselves, namely the permanganate-peroxide titration reaction (widely used to quantify aqueous H_2O_2, both in analytic practice and teaching laboratories). The analysis in Smith & Missen 1990 shows that only the S method predicts the correct physically observed equilibrium (with product species only appearing in given proportions). The NS method predicts a different equilibrium composition (than the single reaction S method considered in Smith & Missen 1990) that is not physically observed.

To further motivate the need for an equivalence proof, and to better understand precisely when equivalence may fail, we provide three additional examples of chemically reactive systems where the S and NS methods are not equivalent in Appendix 2.

3.2. General algebraic proof: S and NS equivalence for the basic gasification problem

The existence of counter examples like the one in section 3.1 prove that the S and NS methods are not necessarily equivalent. In this section we provide the proof that the S and NS methods do become equivalent (will yield the same solutions) for the gasification equilibrium for r large enough, and describe the mathematical computation that can be sued to calculate the critical r^* or number of independent reactions at which the S and NS methods will yield identical solutions.

To do this we will first recall the general algebraic result that stipulates when the S and NS methods will be equivalent. We will then systematically go through the steps necessary to verify that the general algebraic proof applies to the gasification problem as formulated below. (The reader can use the steps here as a template to establish N vs NS equivalence, or the lack thereof, also for any other chemical system, or expanded version of the gasification problem, of interest to the reader).

3.3. Existence and uniqueness

We will in this work assume that both the S and NS problems being considered possess existence and uniqueness. That is, any problem under consideration is assumed to predict a single equilibrium concentration for all species m with all concentrations or partial pressures being positive for all m species. This is generally true for the mathematical models of gasification reactions. For a discussion on how to more rigorously establish the existence and uniqueness for a specific problem see Appendix 7.

3.4. Problem formulation

We will refer to the following chemical system as the **baseline gasification problem**:

Atoms: C, O and H
Molecular species: CO, CO_2, CH_4, H_2O and H_2
Independent chemical reactions: $CO + H_2O \rightleftharpoons CO_2 + H_2$ (WGS)
$CH_4 + H_2O \rightleftharpoons CO + 3H_2$ (SMR)
Problem to be solved: Equilibrium concentrations or partial pressures of the 5 molecular species.

Note: To compute a specific equilibrium composition for a specific scenario the modeler of course also need to specify the following parameters: i) Initial concentrations of all chemical species, ii) the temperature and iii) the total pressure and concentration of inert species like N_2.

It has been repeatedly demonstrated that this formulation of the gasification problem includes all gaseous species present >0.0001 mol% in common application conditions at *complete theoretical equilibrium* [22,29,66–68]. As such this problem statement truly is the relevant homogenous gas phase equilibrium problem that is physically and experimentally relevant to most gasification scenarios. This baseline problem is also not surprisingly either the only, or the core computation, of the vast majority of equilibrium modeling studies published [39].

The NS method requires only that the modeler specifies all the molecular species in the system. The S method alternatively requires the specification of the independent reactions. Here we chose the two shift reactions (WGS = water gas shift & SMR = steam methane reforming) as the independent reactions. The exact choice of which two independent reactions chosen from the larger possible set does not matter since all possible choices will lead to the same S vs NS method equivalence result to be proved here. (For example one can replace the SMR with $CH_4 + 2H_2O \rightleftharpoons CO_2 + 4H_2$, the equivalence result remains the same.) Since the solution to the NS method is unique, and all S method formulations will give identical solutions to the NS method, the proof in this article of S and NS equivalence also establish that the S method solution is the same regardless of the two independent reactions chosen when computing the S method. I.e. a corollary of the rigorous proof here is that the choice of independent reactions in the S problem formulation does not matter – the baseline gasification S problem will yield the identical final equilibrium composition no matter which two independent reactions between the 5 species CO, CO_2, CH_4, H_2O and H_2 is chosen in the problem

formulation and numerical algorithm used to obtain the solution.

Corollary: The S method final solution of the basic gasification problem is independent of the choice of the two independent reactions used for the S method formulation.

Motivation of the homogenous problem formulation. Why not include solid carbon? The formulation of the gasification problem with no solid carbon present specified above represents the situation where either 1) all solid carbon is gasified, or 2) more commonly it is the problem formulation of a researcher that intentionally chooses to only model the gas phase chemical equilibrium between the major (e.g. > 1 vol%) gas phase components. The chosen problem to be solved is calculating the equilibrium distribution of a known amount of C, O and H among the dominant gas-phase components. The amount of carbon, hydrogen and oxygen that is gasified can be accurately determined experimentally from an analysis of the feedstock, and an analysis of the residual char and ash (and tar gasses and/or tar condensate in cases where the tar is not negligible) [43]. It certainly is easy to expand the equilibrium problem to the heterogeneous equilibrium by adding solid carbon or some solid model compound, and a heterogeneous reaction. Many modelers indeed have chosen three independent reactions from the heterogeneous system that include "solid C" as their S model reactions. The equivalence results of this paper can be rigorously expanded to this situation. However, it is useful to keep in mind that although one can try to estimate the amount of solid carbon that will be gasified theoretically (at complete heterogeneous equilibrium) this prediction frequently might be of limited use because firstly the chemical configuration (and hence standard Gibbs energy of formation) of the solid feedstock is rarely simple (i.e. solid carbon in typical biomass, coal etc. is not predominantly just a single chemical species with single precisely known molecular structure and Gibbs energy) and secondly complete heterogeneous thermodynamic equilibrium is hard to attain in realistic gasifiers [17]. Hence, the literature confirms that it is indeed difficult to make the alternative heterogeneous problem, where one includes solid carbon as an additional species and add a third heterogeneous reaction to the list of reactions, thermodynamically relevant to an actual application without empirical fudge factors.

4. Result from linear algebra

The proof that the S and NS methods are equivalent for any reactive system utilizes the following basic result of liner algebra [69]:

4.1. Rank-nullity theorem

For any matrix A it is always true that
$\text{rank}(A) + \text{null}(A) = \text{col}(A)$

where $\text{null}(A)$ is the 'nullity' or dimension of the nullspace or kernel of A, $\text{col}(A)$ is the number of columns in A, and $\text{rank}(A)$ has the usual definition, namely the number of linearly independent columns of A.

In the context of computing the equilibrium composition of a reacting chemical system this result becomes (For a rigorous proof see Appendix 3 or Smith 1980 [70]):

4.2. Criterion for equivalence

S vs. NS Equivalence Theorem
The S and NS methods are equivalent
if and only if
1) $r = \text{null}(A) = m - \text{rank}(A)$
where
2) r is the number of algebraically independent reactions in the S problem formulation

Here A is the formula matrix $\{a_{ki}\}$, where a_{ki} is number of atoms of type k in molecular species i. I.e. we label the atom types in the system as $k = 1, 2, \cdots, n$ and the molecular species $i = 1, 2, \cdots, m$. r is the number of reactions (specified in the formulation of the S problem) and m is the number of molecular species (specified in the formulation of the NS problem), that is $m = \text{col}(A) =$ number of columns of matrix $A =$ number of molecular species .

Note that although $\text{rank}(A)$ frequently is equal to the number of elements n, it is true for some systems that $\text{rank}(A) < \text{row}(A) =$ number of elements. Unlike in the analysis here, or in Smith 1980 [70], this fact is unfortunately omitted or neglected in some widely used textbooks and relevant reference works, for example [71,72].

We observe that the theorem settle, with rigorous algebra, the question "how many independent reactions" are required to achieve any possible redistribution of the atoms in our system between the molecular species in our system. The algebraic answer is that the number of reactions (or balanced stoichiometric vectors) r^* that span the space of all atomic redistributions equals the dimension of the nullspace of the formula matrix A. Finally, the rank-nullity theorem simply provides a convenient algebraic formula for computing the dimension of the nullspace of A.

If our S method formulation has less independent reactions than $\text{null}(A)$, i.e. if $r < \text{null}(A)$, then the methods are not equivalent. If our S method formulation has $r = \text{null}(A)$, then the S and NS methods are equivalent. Finally, we note that $r > \text{null}(A)$ is mathematically *impossible* for linearly independent reactions, since by definition $\text{null}(A)$ is the *dimension* of the nullspace. I.e. the maximum number of linearly independent (reaction) vectors that can possibly exist is $\text{null}(A)$ and we always have $r \leq \text{null}(A)$ for any set of linearly independent reactions in the S method formulation.

We will now apply this result to the gasification problem in three steps. (We will write out these admittedly simple steps explicitly so that the presentation in this technical review can serve as a clear template for establishing equivalence in other applications where these particular steps may be less trivial.)

Step 1 – Rank of A matrix

The formula or A matrix in the basic homogenous/gas phase gasification problem for our problem formulation is:

$$\begin{array}{c} \\ \text{C} \\ \text{O} \\ \text{H} \end{array} \begin{array}{c} \begin{array}{ccccc} \text{CO} & \text{CO}_2 & \text{CH}_4 & \text{H}_2\text{O} & \text{H}_2 \end{array} \\ \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 2 & 0 & 1 & 0 \\ 0 & 0 & 4 & 2 & 2 \end{bmatrix} \end{array}$$

It is easy to verify, using for example row reduction, that $\text{rank}(A) = 3$.

Step 2 – Independence of reactions

The stoichiometric matrix $\bar{\bar{\nu}}$ for our reactions is:

$$\begin{array}{c} \\ \text{CO} \\ \text{CO}_2 \\ \text{CH}_4 \\ \text{H}_2\text{O} \\ \text{H}_2 \end{array} \begin{array}{c} \begin{array}{cc} \text{WGS} & \text{SMR} \end{array} \\ \begin{bmatrix} -1 & 1 \\ 1 & 0 \\ 0 & -1 \\ -1 & -1 \\ 1 & 3 \end{bmatrix} \end{array}$$

Clearly we have two independent columns and hence two algebraically independent reactions.

Step 3 – Equivalence criterion

Thus far we have $\text{rank}(A) = 3$, $r = \text{rank}(\bar{\bar{\nu}}) = 2$ and $m = \text{col}(A) =$

5.

Hence we have $r = m - \text{rank}(A)$, and we can definitively and rigorously conclude that the S and NS methods are equivalent for the gasification problem as formulated above. The equilibrium composition predicted by these two methods will be identical.

4.3. Specific proof: S and NS equivalence for the basic gasification system

The algebraic proof just provided is succinct, general and rigorous. However, it is also somewhat abstract. Some readers may prefer or find benefit in a more concrete prove since such a proof may provide some intuition as to the physical structure and constraints present in the gasification scenario.

For example, note that the domain over which both the S and NS methods minimize the Gibbs energy is just like that shown in Fig. 2, i.e. that it is essentially 2 dimensional can be easily seen by considering Fig. 3 and the following: Atoms are conserved in both methods (a column vector $\bar{\nu}$ of $\overline{\nu}$ must be in the nullspace of A since all non-nuclear reactions conserve atoms). Once the amount of CO and CO_2 in the product stream (final equilibrium) is specified, the carbon balance immediately implies the amount of CH_4. Likewise, the oxygen atom balance immediately implies the amount of residual H_2O. Finally, since the amount of CH_4 and H_2O is already set for a given a choice of CO and CO_2, the amount of H_2 is also fixed by the hydrogen balance. I.e. there are only two degrees of freedom. For example, choose the final amounts of CO and CO_2 and the final amounts all other chemical species are also set by the elemental balances.

We can use this reduction in dimension of the gasification problem, together with the non-negativity conditions on chemical species, to construct a second, perhaps less abstract proof that the S and NS methods are equivalent for the gasification problem. Since it may provide intuition into the structure and constraints of the gasification problem, we provide this alternative proof in Appendix 4.

4.4. S vs NS advantages and a common error in the literature

Does the initial composition used in the S method matter? More precisely, would changing the distribution of the given amounts of each element in the system between the species m in the inlet feed change the final equilibrium composition? (Recall that we are considering the isothermal problem.) We already know that the answer is no for the NS method. As a corollary to this proof, and the fact that the S & NS methods yield identical results, one can immediately see that the initial composition used to compute the S method solution also does not matter (whenever $r = 2$, for an alternative S model with $r < 2$ the final answer will become dependent on the initial composition). More precisely, the initial distribution of a given amount of C, H and O atoms between the 5 species used in the S method (CO, CO_2, CH_4, H_2O and H_2) does not alter the final S method solution (with any two independent reactions between the 5 species). The equilibrium distribution predicted by both methods remain the same regardless of the initial distribution chosen in the S method as long as that initial distribution preserve the atom totals. (This holds for the isothermal problem in this article. For the adiabatic problem a different initial composition result in a different final temperature in both methods. I.e. the two methods still lead to identical solutions in the adiabatic problem, but, that identical solution now change with the initial composition since the final temperature does.) The fact that changing the initial composition (distribution of atoms among allowed species) does not change the final equilibrium (for the adiabatic problem) only becomes clear once one become aware of the equivalence proof. There is, as a consequence, a relatively common mistaken notion prevalent in the literature for example expressed as "one advantage of the NS method over the S method is that the S method requires precise knowledge of the initial composition, while the NS method only requires precise knowledge of CHO totals". E.g Ref. [45,47,52,55,58,59]. Given the equivalence proof here and its corollary, one can see that the notion in the literature that there is an inherent advantage in the NS method over the S method related to "the need to specify initial distributions" is not correct. For both methods one *does need to know* the C, H, and O *atom totals* in the system accurately, but the precise initial distribution is irrelevant and does not alter the S method (or identical NS method) answer whatsoever (assuming of course consistent and stable numerical algorithms for both methods so that both will converge to the same unique mathematical solution). Any initial distribution will yield the same unique answer. (For the adiabatic case, both methods require an accurate initial composition to compute the final temperature, so again there is no inherent accuracy advantage of one method over the other.)

In conclusion, there is no mathematical accuracy advantage, or 'need to know more information' advantage or disadvantage between the two methods. The only possible advantage could be the relative stability or simplicity of the numerical algorithm employed.

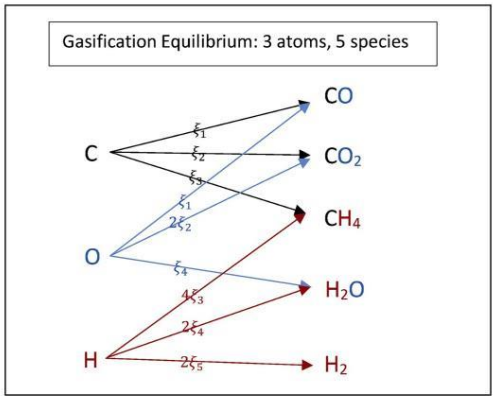

Fig. 3. The basic gasification problem is the distribution of C, O and H between 5 products. Given the atomic balances the degrees of freedom remaining is two, i.e. the Gibbs energy is minimized over a two-dimensional domain.

5. Conclusions

A technical review of the gasification modeling literature revealed a roughly 50-50 disagreement in gasification equilibrium modeling work to date; one camp states that the S and NS approaches will yield the same results, while the other camp suggest that the two approaches will yield different equilibrium compositions with one or the other approach being superior.

The subset of articles that suggest that the S and NS approaches yield identical equilibrium compositions for the basic gasification problem is correct. However, none of the works reviewed, and none of the 9 prior reviews of the gasification modeling and simulation literature published [1,6,7,14,23,24,30,47,73], contain a valid definitive proof (or reference to a proof) of the equivalence of the S and NS methods. To rectify this situation a rigorous proof of the S and NS method equivalence for the basic gasification equilibrium problem was presented in section 3 of this technical review. The proof shows that the stoichiometric (S) method and the non-stoichiometric (NS) method will always yield identical results for the baseline homogenous gas phase gasification equilibrium.

In addition to providing a resolution to the disagreement in the existing literature the systematic proof here also provides a template that can be used to establish equivalence or non-equivalence of the S vs NS methods for other systems of reactions and chemical species, this could be an extended or more elaborate formulation of the gasification

problem or any other reactive system. For example, although the concentrations of radical species are by definition small, the equilibrium amounts of radical or intermediate species are of interest in certain studies [74–76]. This will add additional molecular species (for example OH* and/or H*) and reactions to the system model. The theorem and template presented here can be used to check whether any expanded chemical system with additional radical species and elementary reactions included constitutes a system with S and NS equivalence, or conversely, constitutes a case where $r < r^*$ so that the two approaches could predict different radical concentrations at equilibrium.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

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Paper IV

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Abstract

Biomass is one of the most widely available energy sources and gasification is a thermal conversion process where biomass is transformed into a fuel gas with a gasifying agent. In this paper by using ASPEN Plus, a new steady state simulation model for down draft waste biomass gasification was developed. The model that is stoichiometric equilibrium-based is proposed to be used for optimization of the gasifier performance. Prediction accuracy of the model is validated by comparing with available experimental and modeling results in other literature. Then the model is used for comparative analysis of the gasification performance of sawdust, wood chips and mixed paper wastes. In the model, the operating parameters of temperature and equivalence ratio (ER) have been varied over wide range and their effect on syngas composition, syngas yield, low heating value (LHV) of syngas and cold gas efficiency (CGE) has been investigated. Raise in temperature increases the production of CO and H_2 which leads to higher syngas yield, LHV and CGE. However, increasing ER decreases the production of CO and H_2 which results lessens in LHV and CGE but syngas yield continuously increases because more oxygen is available for biomass reactions at high ER. The optimal values of CO and H_2 mole fraction and CGE of sawdust, wood chips and mixed paper wastes are located at 900˚C, 1000˚C and 1000˚C, respectively and ER range is between 0.20 - 0.35 regardless of the kind of biomass which is used as the feedstock.

Keywords

Waste Biomass Gasification, Simulation Model, Gasifier Performance, Waste to Energy

1. Introduction

Negative impacts of fossil fuels on social, political and environmental aspects as well as energy security concerns have encouraged the interest in nonpetroleum energy sources [1] [2]. Among the various alternative energy sources, biomass has obtained more interest since it is the only suitable and renewable primary energy resource that can provide alternative transportation fuels [3] [4] [5]. Extracting energy from biomass requires biochemical or thermochemical processes [6]. During biochemical processes, biomass is converted to biogas and residual by the digestive action of living organisms. However, in thermochemical processes like gasification, biomass is converted to biofuels, gases and chemicals by applying heat and pressure. Gasification is also characterized by higher temperatures and conversion rates than biochemical and thermochemical processes, so allowing an efficient treatment of various types of biomass wastes. In addition to producing syngas from biomass for subsequent biofuel synthesis gasification typically achieves superior efficiency for electricity generation from biomass compared to more conventional alternatives like incineration. Electricity production by using gasification, extracts more electricity per kilogram biomass, or per kilogram municipal waste [7] [8] [9] [10], compared to alternatives like incineration or biogas from digesters [11].

The gasification process consists of drying, pyrolysis, combustion and gasification. Drying occurs at a temperature between 100˚C - 150˚C, pyrolysis is in the range of 200˚C - 700˚C, combustion occurs in 700˚C - 1500˚C and gasification is in the range of 800˚C - 1100˚C [12]. Typically, the moisture in biomass ranges from 5% to 35% that it is reduced to lower 5% during drying. In the pyrolysis step, the volatile components in the biomass are vaporized as it is heated in the absence of oxygen. The volatile vapor is a mixture of hydrogen, carbon monoxide, carbon dioxide, methane, hydrocarbon gases, tar and water vapor [13]. At the next step, oxygen supplied to the gasifier reacts with the combustible substances, resulting in CO_2 and H_2O, which subsequently undergo reduction upon contact with the char produced from pyrolysis [12]. Reduction yields combustible gases like hydrogen, carbon monoxide and methane through a series of reactions, the main reactions in this category are in below [11] [14] [15].

In reviewing past studies, attempts in simulating biomass gasification have been carried out to evaluate the gasification performance affected by various operating conditions. The simulations of biomass gasification can be divided into kinetic rate models and thermodynamic equilibrium models. In comparison to kinetics approaches, thermodynamic equilibrium calculations have fewer complexities and independent of gasifier design, so it makes them suitable for studies on the influence of fuel process parameters [11].

The composition of a mixture at thermodynamic equilibrium can be estimated using different methods of stoichiometric and non-stoichiometric approaches. When implementing the stoichiometric method, a set of independent chemical reactions are specified, thereafter the initial concentrations of all

chemical species are specified, and the equilibrium concentrations are then calculated by solving for the extent of every reaction. However, when implementing the non-stoichiometric method, no reactions are specified and the concentrations of the species are evaluated to minimize the Gibbs energy of the products, in accordance with the constraints imposed by the principle of conservation of mass and of the stoichiometry [16]. Numerous researchers have focused on the non-stoichiometric method for biomass gasification because for this method does not need a detailed specification of all the chemical reactions taking place in the reactor. Our recent review [11] of studies reporting the modelling of biomass gasification suggests that up to May 2018 approximately 27.5% of gasification modeling studies use the stoichiometric method, roughly 72.5% use the non-stoichiometric method and no published study uses both methods to solve the same problem. However, it is worth mentioning that the authors are not aware of any published simulation study on biomass gasification systems based on the stoichiometric method.

Hence, the objective of this study is to develop a stoichiometric steady state computer model for waste biomass gasifier using the simulation software ASPEN Plus. Then the model is applied to evaluate and compare the gasification performance of three different feedstocks; *i.e.*, wood chips, sawdust and mixed paper waste as the significant municipal organic wastes. Finally, the effect of operating parameters like temperature and equivalence ratio (ER) on the main indicators of performance evaluation of gasification system like syngas composition, syngas yield, low heating value (LHV) of produced syngas and cold gas efficiency (CGE) are investigated to find the optimal conditions.

2. Material and Methods

2.1. Simulation Model

A new kinetic free equilibrium model based on stoichiometric approach has been developed for the downdraft air gasifier of waste biomasses by using ASPEN Plus version 10. In this study, the developed Aspen Plus model involves the following steps: specification of stream class, selection of property method, determination of the system component from databank, specification of the conventional and non-conventional components, Specifying the process flowsheet by using unit operation blocks and connecting material and energy streams, defining feed streams (flow rate, composition, and thermodynamic condition) and Specifying unit operation blocks (thermodynamic condition, chemical reactions, etc.).

2.1.1. Assumptions

The following assumptions are employed in the simulations of waste biomass gasification.

1) The model is at steady state, kinetic free and isothermal.

2) All gases are ideal gases, including hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), steam (H_2O), nitrogen (N_2) and methane (CH_4).

3) Char contains only carbon and ash in solid phase.

4) Tar and other heavy hydrocarbons are not considered.

5) Operation at atmospheric pressure (~1 bar).

6) No heat and pressure losses occur in the gasifier.

7) Simulation is based on stoichiometric approach and by considering reactions of R1, R2, R4, R5 and R7 in **Table 1**.

2.1.2. Physical Property Method

According to our conducted review, about 30% of studies employed Peng Robinson as the physical property method for simulation of biomass gasification (**Table 2**). However, approximately 44% of researches have not talked about the applied physical property method. Hence in our work, Penge Robinson equation of state with Boston-Mathias alpha function (PR-BM) has been used to estimate all physical properties of the conventional components in the gasification process. This method is suitable for the nonpolar or mildly polar mixtures such as hydrocarbons and light gases and the parameter alpha in this property package is a temperature dependent variable that could be helpful for the correlation of the pure component vapor pressure when temperature is quite high. Moreover, the enthalpy and density model selected for both biomass and ash which are non-conventional components are HCOALGEN and DCOALIGT. MCINCPSD stream containing three substreams comprising MIXED, CIPSD and NCPSD class, was also used to define the structure of simulation streams for the components of biomass and ash which are not available in the standard Aspen Plus component database.

Table 1. Main gasification reactions [11] [14] [15].

Heterogeneous reactions		
$C + O_2 \rightarrow CO_2 + 394\ kJ/mol$	Complete combustion	R1
$C + H_2O \rightarrow CO + H_2 - 131 kJ/mol$	Partial combustion	R2
$C + CO_2 \rightarrow 2CO - 172 kJ/mol$	Boudouard	R3
$C + H_2O \rightarrow CO + H_2 - 131 kJ/mol$	Water-gas	R4
$C + 2H_2 \rightarrow CH_4 + 75 kJ/mol$	Methanation	R5
Homogeneous reactions		
$CO + 0.5O_2 \rightarrow CO_2 + 283 kJ/mol$	CO partial combustion	R6
$H_2 + 0.5O_2 \rightarrow H_2O + 242 kJ/mol$	H2 combustion	R7
$CO + H_2O \rightarrow CO_2 + H_2 + 41 kJ/mol$	CO shift	R8
$CH_4 + H_2O \rightarrow CO + 3H_2 - 206 kJ/mol$	Reforming	R9
H2S and NH3 formation reactions		
$H_2 + S \rightarrow H_2S$	H2S formation	R10
$3H_2 + N_2 \rightarrow 2NH_3$	NH3 formation	R11

Table 2. Physical property methods selected by various researches.

Redlich Kwong Soave with Boston Mathias modifications (RKS-BM)	Penge Robinson with Boston-Mathias alpha function (PR-BM)	Peng-Robinson	IDEAL	Model not mentioned
Paviet *et al.* 2009 [17], Begum *et al.* 2014 [18], Pardo-planaz *et al.* 2017 [19], Eikeland *et al.* 2015 [20], Eikeland and Thapa 2017 [21], Guruprasad *et al.* 2014 [22]	Ramzan *et al.* 2011 [23], Formica *et al.* 2016 [6], Pala *et al.* 2017 [24], Sun 2015 [25], Fernandez-Lopez 2017 [26], Xiangdong *et al.* 2013 [27]	Kuo *et al.* 2014 [28], Gagliano *et al.* 2017 [29], Lestinsky and Palit 2016 [30], Damartzis *et al.* 2012 [31]	Han *et al.* 2017 [32]	Doherty *et al.* 2008 [33], Doherty *et al.* 2009 [34], Keche *et al.* 2015 [35], Mavukwana *et al.* 2013 [36], Rupesh *et al.* 2016 [37], Dahmani *et al.* 2017 [38], Deng *et al.* 2017 [39], Nikoo and Mahinpey 2008 [40], Panda 2012 [41], Peters *et al.* 2017 [42], Kaushal and Tyagi 2017 [43], Abdelouahed *et al.* 2012 [44], Mathieu and Dubuisson 2002 [45]

2.1.3. Model Description

Figure 1 shows the flow chart of waste biomass gasification simulation by using ASPEN Plus based on the stoichiometric approach and **Table 3** gives the brief descriptions of the unit operations of the blocks used in the simulation. The BIOMSS stream was defined as a nonconventional stream and it was created by inputting of elemental and gross compositions of wastes feedstocks obtained from proximate and elemental analyses. The information used to describe the feedstocks is given in **Table 4**. In the next step, RYIELD, the ASPEN Plus yield reactor, was used to simulate the decomposition of the feed. In pyrolysis/decomposition stage, the feedstock was transformed from a non-conventional solid to volatile materials and char. The volatiles included carbon, hydrogen, oxygen and nitrogen and the char was converted into ash and carbon, by specifying the product distribution based on the proximate and ultimate analysis of the waste biomasses. The yield of volatiles was equal to the volatile content in the fuel according to the proximate analysis [28] [31] [40]. For stoichiometric equilibrium simulation of the combustion and gasification parts, REquil reactor was used in which homogeneous and heterogeneous reactions can be defined, simultaneously. However, due to the limitation of ASPEN Plus that each REquil can only contain one heterogeneous reaction, 4 REquil reactors (RE1-RE4) were considered for 4 heterogeneous reactions of R1, R2, R4, R5 (based on **Table 1**). Two FSplit blocks were used for dividing of volatiles and air streams among reactors of RE1, RE2 and RE3. Then two Mixer blocks were applied to mix outlet gasses and unburned carbons from the up and bottom of reactors, respectively; the product streams called OUTGAS and CARBON, respectively. Then, OUTGAS and CARBON streams with the rest of air stream were entered to RE4 for the heterogeneous reaction of R5 and homogenous reaction of R7. Eventually, the product gas called SYNGAS was exited from the up of RE4.

Table 3. Description of ASPEN Plus unit operation blocks used in model.

ASPEN Plus name	Block name	Description
Ryield	PYROL	Decomposition of non-conventional biomass to conventional components according to its proximate and ultimate analyses.
Requil	RE1, RE2, RE3, RE4	Rigorous equilibrium reactor based on stoichiometric approach.
Sep	SEPRATOR	Gas separation from ash by specifying split fractions.
FSplit	S1, S2	Dividing of gas stream and air stream based on split fractions by S1 and S2, respectively.
Mixer	M1, M2	Blending of gasses and carbons into one stream by M1 and M2, respectively.

Table 4. Ultimate and proximate analysis feedstocks.

Feedstocks	Sawdust	Wood chip	Mixed paper waste
Proximate analysis			
Proximate analysis (*wt*%)			
Moisture	7	20	8.8
Volatile matter (VM)	81.72	80	84.2
Fixed carbon (FC)	17.2	18.84	7.5
Ash	1.08	1.16	8.3
Ultimate analysis			
Elemental analysis (*wt*%-*dry basis*)			
C	46.46	51.19	47.96
H	5.82	6.08	6.60
N	0.19	0.2	0.18
O	46.45	41.37	36.96

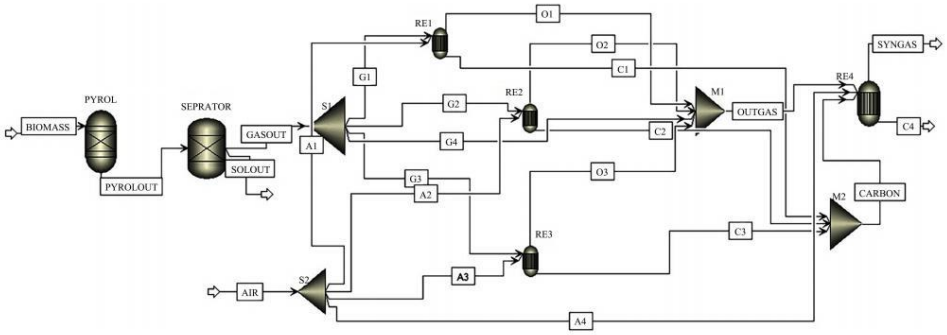


Figure 1. Flow chart of waste biomass gasification simulation using Aspen Plus.

3. Validation

In order to validate the present model, the syngas composition obtained through gasification from the developed simulation model have been compared with the experimental data published by Jayah (2002) [46] and with the thermodynamic analyses based on non-stoichiometric of Paviet *et al.* (2009) [17]. They conducted air gasification of rubber wood as biomass feedstock in a down draft gasifier. **Figure 2** shows the results of comparison at temperature of 1300 K and air to fuel ratio of 2.53. It can be observed that the present model shows better agreement with the experimental results compared to the non-stoichiometric based model. Only formation of methane was underestimated by the model which is quite a common problem for equilibrium models that cannot predict much more hydrocarbons (especially methane) [17] [24] [34].

The stoichiometric thermodynamic model of gasification was also validated by comparing the current predictions to the experimental results of Jayah *et al.* [47]. In their work, rubber wood was considered as feedstock into a down draft gasifier operated at atmospheric pressure and the gasification temperature of 900˚C. Six different air to fuel mass flow rate ratios (AFRs) were considered and the comparisons of CO, H_2, CO_2 and N_2 concentrations were shown in **Figure 3**. The deviation of the model results from experimental values is quantified by using statistical parameter RMS (root mean square) error. The maximum RMS error of 1.89 is obtained when six sets of experimental data are compared with the corresponding model values for syngas composition.

4. Results and Discussion

In this study, the developed model for waste biomass gasification has been used to investigate the gasification performance of three different waste feedstocks: sawdust, wood chips and mixed paper waste. The effect of gasifier temperature and equivalence ration (ER) on syngas composition, syngas yield, lower heating value (LHV) of produced gas and cold gas efficiency (CGE) has been investigated. Syngas yield in this model is the volume of total product gas from the gasification per unit weight of fuel in normal conditions (Nm^3 kg $fuel^{-1}$). The lower heating value of product gas is calculated as [28] [48]:

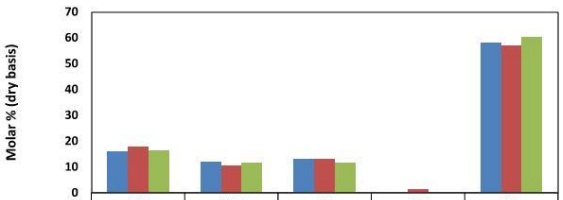
$$\mathrm{LHV_{syngas}}\left(\mathrm{kj/Nm^3}\right)=4.2\times\left(30\times y_{CO}+25.7\times y_{H_2}+85.4\times y_{CH_4}\right) \quad (1)$$

where y is the mole fraction of gas pieces in the syngas (dry basis).

The cold gas efficiency (CGE) is an important index to account for the performance of biomass gasification that it is calculated by using Equation (2) [28] [49]:

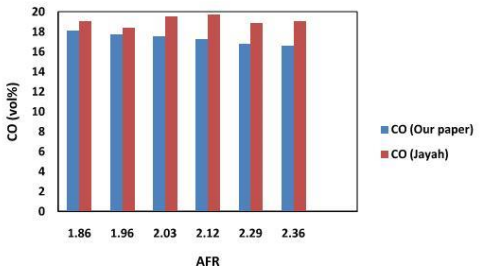
$$\mathrm{CGE}(\%)=\frac{\mathrm{G_P}\times\mathrm{LHV_{syngas}}}{\mathrm{HHV_{fuel}}}\times 100 \quad (2)$$

where GP is the syngas yield and $\mathrm{HHV_{fuel}}$ is the higher heating value of fuel (MJ kg $fuel^{-1}$) that it is calculated by below equation [50].

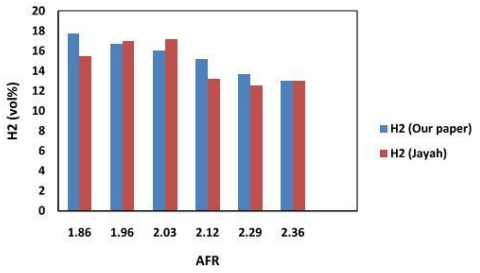


	CO	CO2	H2	CH4	N2
Paviet 2009	16	12	13	0	58
Jayah 2002	18	10.5	13	1.5	57
Our paper	16.24904283	11.65441956	11.76288822	0.007562318	60.32608707

Figure 2. Comparisons of syngas composition between our model and Jayah (2002) [46] experimental measurements and Paviet *et al.* (2009) [17] model.



(a)



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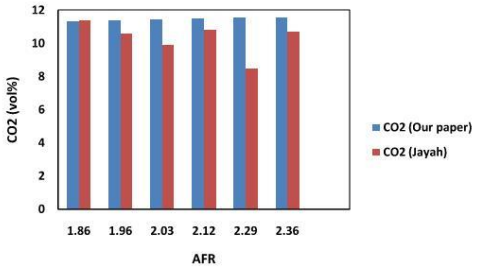

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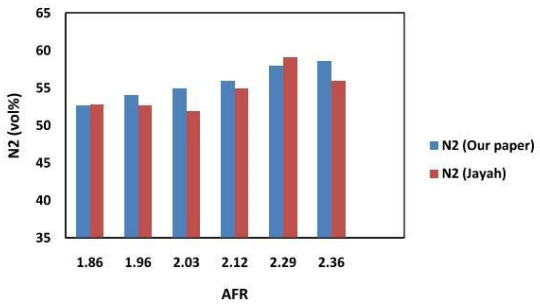


(d)

Figure 3. Comparisons of (a) CO, (b) H_2, (c) CO_2 and (d) N_2 concentrations between stoichiometric predictions and experimental measurements.

$$\mathrm{HHV}_{\mathrm{fuel}}\left(\mathrm{Mj/kg}\right)=0.312\times\left(\mathrm{FC}\right)+0.1534\times\left(\mathrm{VM}\right) \tag{3}$$

According to the Equation (3), heating value is a function of weight fractions of fixed carbon and volatile matter in the dry and ash-free conditions.

4.1. Effect of Temperature on Syngas Composition

The effect of gasifier temperature on syngas mole fractions for three feedstocks was examined in the window of 500˚C - 1500˚C, while all the remaining operating conditions were fixed. As shown in **Figure 4**, at very low temperature of 500˚C the existing carbon in the biomass is not used completely, so the syngas production would not be in a good rate. In such a low temperature, unburned carbon and methane will remain in syngas while by increasing temperature more carbon is oxidized and converted to carbon monoxide in accordance with partial combustion reaction (R2). Methane is also transferred into hydrogen by reverse methanation reaction (R5). Moreover, at high temperature, water gas reaction (R4) goes toward the production of both carbon monoxide and hydrogen. Hence, increasing the gasifier temperature favors hydrogen and carbon monoxide production, leads to the improvement of heating value of syngas (based on Equation (1)). However, at a specific temperature, yield of H_2 and CO reach to an approximately fixed points that this point can be the optimum gasifier temperature for each waste. The optimum operating temperature of the down draft gasifier for sawdust, wood chips and paper wastes are 900˚C, 1000˚C and 1000˚C, respectively. Methane production also decreases sharply at temperatures above 600˚C for three wastes. For both sawdust and wood chips wastes, mole fraction of CO is higher than H_2 mole fraction but general behavior is not the same for paper waste. According to the elemental analysis of feedstocks, mixed paper waste has the highest hydrogen and the lowest oxygen among the others, consequently the product gas from paper gasification includes lower CO but higher H_2 in comparison other wastes.

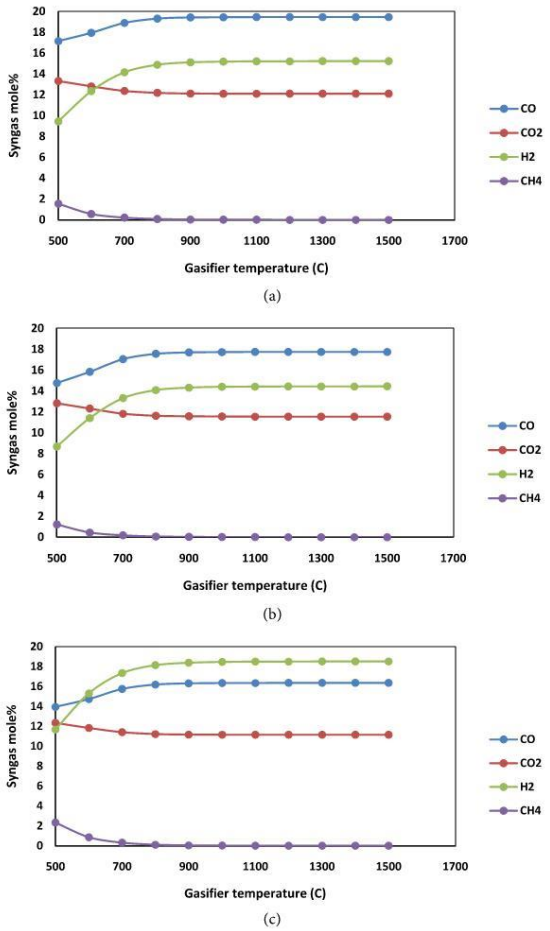


Figure 4. Effect of temperature on syngas mole fraction (dry basis), (a) sawdust, (b) wood chip, (c) mixed paper waste.

4.2. Effect of ER on Syngas Composition

Equivalence Ratio (ER) is an important index for showing the role of oxidizing agent and it is defined as the ratio of the amount of actual air supplied to the gasifier to the stoichiometric air. At low ER, biomass reactions will approach to the pyrolysis, whereas at a high ER the excess amount of oxygen oxidizes the fuel completely and causes biomass combustion; then the production of syngas declines. Hence, it is important to find the appropriate range of ER for biomass gasification that has been studied in this work. In this case, the ER in the gasifier was varied from 0.1 - 0.7 and its influence on the syngas compositions were

shown in Figure 5 for three wastes. The H_2 mole fraction decreases with increasing ER, regardless of which biomass is used as the feedstock. Similar to H_2 formation, the mole fraction of CO also decreases with increasing ER but an opposite trend for CO_2 is exhibited. This is due to when ER rises, more oxygen is supplied for biomass reactions, so fuel goes toward the full combustion. Sawdust has highest mole fraction of carbon monoxide and hydrogen in syngas (0.28 and 0.38, respectively). Conversely, the gasification of mixed paper waste gives the lowest mole fraction of CO (0.22). Finally, as shown in Figure 5 the optimum ER lies between 0.2 - 0.35 for three wastes (till mole fractions of carbon monoxide and hydrogen are higher than 20%).

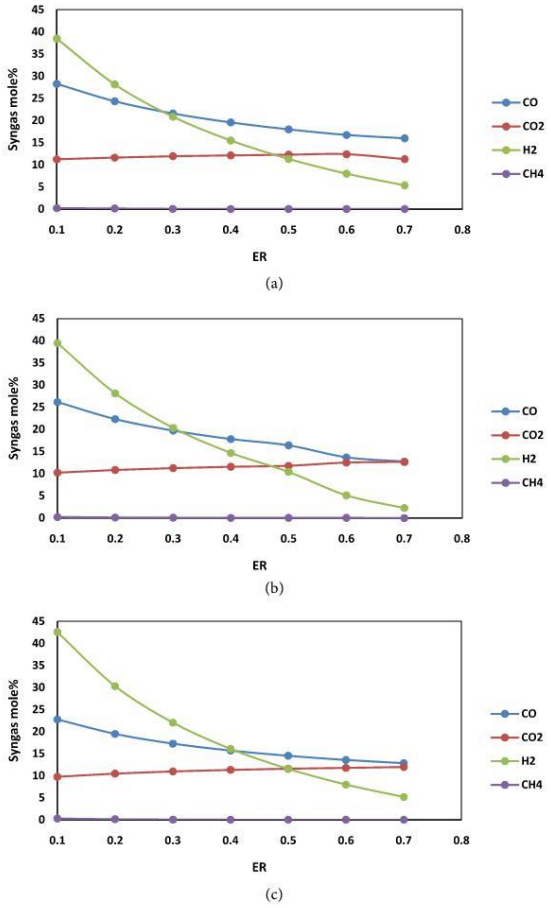
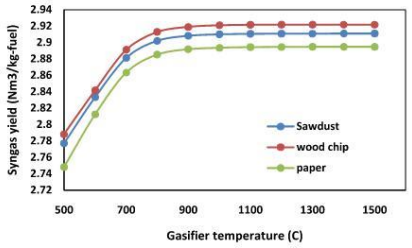


Figure 5. Effect of ER on syngas mole fraction (dry basis), (a) sawdust, (b) wood chip, (c) mixed paper waste.

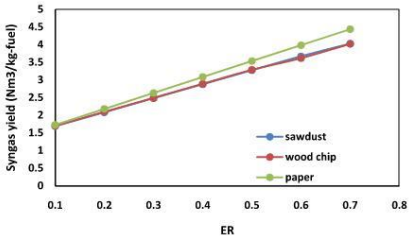
4.3. Effect of Temperature and ER on Syngas Yield

The effect of the gasifier temperature on the syngas yield is illustrated on **Figure 6(a)**. When the operating temperature of gasifier is increased from 500˚C - 900˚C, the syngas yield is increased 4.6% for sawdust and wood chips and 5.4% for mixed paper waste and then reach to approximately fixed points. It can be explained by increasing gasifier temperature, the unburned carbon is converted into carbon monoxide and through the reverse methanation reaction, methane is converted into hydrogen. Finally, mole fractions of components attain to the constant amounts that cause nearly constant values for syngas yield. **Figure 6(a)** depicts that the syngas yield for wood chips gasification is higher than other wastes, because syngas production from gasification of wood chips waste has highest carbon monoxide and hydrogen due to high percentage of carbon and hydrogen in wood chips biomass (as shown in **Table 4**).

The variation of syngas yield for three wastes by varying ER is shown in **Figure 6(b)**. The syngas yield from the gasification of paper waste is higher than that of wood chip and sawdust wastes averagely 7.3%. As ER increases from 0.1 to 0.7, syngas yield continuously increases because more oxygen is available for biomass reactions at high ER but so high syngas yield does not mean high gasification performance. Because as it was explained in Section 4.2, with access to more oxygen, the fuel is oxidized completely and causes biomass combustion; then the production of CO and H_2 decline and CO_2 production increases. In the optimum range of ER, syngas yield values for sawdust, wood chips and paper wastes are in the span of 2.08 - 3.00 Nm^3 $kg\ fuel^{-1}$.



(a)



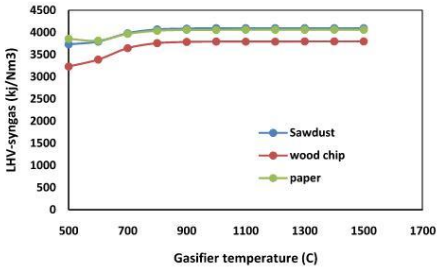
(b)

Figure 6. (a) Effect of temperature on syngas yield; (b) Effect of ER on syngas yield.

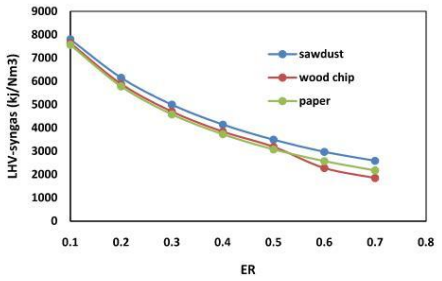
4.4. Effect of Temperature and ER on LHV

Figure 7(a) shows the lower heating value of syngas as a function of temperature. The increase in temperature of the gasification zone at fixed AFR of 2.03 results in an increase in the LHV of the syngas till a specific temperature that is called optimum temperature. LHV values for sawdust, wood chips and mixed paper wastes at optimum temperatures (900˚C, 1000˚C and 1100˚C, respectively) are about 4.09, 3.79 and 4.06 Mj·Nm^{-3}, respectively. Wood chip shows lowest heating value among the three wastes due to relatively lower dry basis mole fraction of carbon monoxide and hydrogen in the syngas. The production of carbon monoxide and hydrogen is dependent on the biomass composition and it is clear from the composition of feedstocks provided in **Table 4** that although wood chip has highest percentage of carbon, it includes so high amount of moisture. Moisture content indirectly effects on LHV of syngas. Increasing moisture content strongly degrades the syngas LHV. As a consequence of much higher moisture content in the fuel, the percentage of carbon and hydrogen in wet basis decrease then leads to lower production of carbon monoxide and hydrogen in the syngas.

The sensitivity of ER over the LHV of the product syngas at the fixed gasifier temperature of 900˚C for three waste biomasses is shown in **Figure 7(b)**. By



(a)



(b)

Figure 7. (a) Effect of temperature on syngas LHV; (b) Effect of ER on syngas LHV.

increasing ER, the production of carbon monoxide and hydrogen in syngas decrease due to complete combustion of fuel, so the heating value of the syngas decreases. As a whole, the LHV of the product gas depends strongly on ER and it is in the range of 4.15 and 6.147 $MJ \cdot Nm^{-3}$ In the optimum range of ER. On the other hand, the effect of feedstock on LHV is slight.

4.5. Effect of Temperature and ER on CGE

Cold gas efficiency is the most crucial parameter that practically indicates the economic efficiency of the gasifier. Accordance to Equation (2), CGE is dependent on different parameters of syngas yield, HHV of fuel and LHV of syngas, but it eventually depends on the amount of carbon monoxide, hydrogen and methane in the product syngas. The composition of syngas is also controlled by temperature and ER hence they are the important parameters for evaluating of CGE. In our model temperature has been varied from 500˚C - 1500 ˚C and the corresponding CGE is calculated. The results have been depicted in **Figure 8(a)**. Mixed paper waste shows highest CGE (70.6%) at temperature of 1000˚C while for sawdust CGE is maximum around 65,8% and wood chips shows lowest CGE (60%) among the three wastes. **Figure 8(b)** shows that increasing ER reduces the value of CGE, stemming from the reduction of LHV (**Figure 7(b)**). For the three waste biomasses, the amount of CGE is under 60% as long as ER is more than 0.4. It follows that ER should be controlled below 0.4.

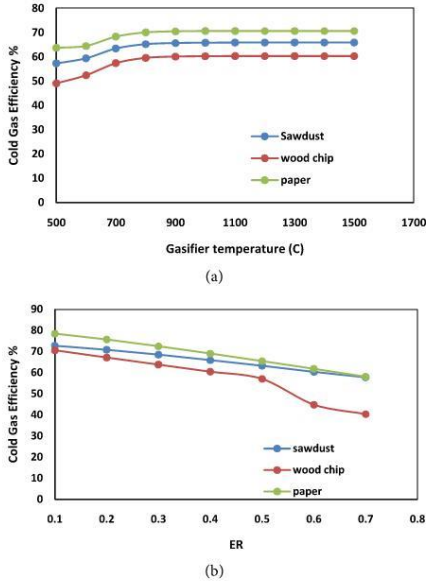


Figure 8. (a) Effect of temperature on CGE; (b) Effect of ER on CGE.

5. Conclusions

A new steady state stoichiometric equilibrium-based model was developed for waste biomass gasification using ASPEN Plus simulator. Prediction accuracy of the model was checked by comparing with available experimental and modeling results in other researches. Then the model was used for comparative analysis of the gasification performance of sawdust, wood chips and mixed paper wastes. In the model, sensitivity analysis was performed and the impact of varying gasifier operating temperature and ER on syngas composition, syngas yield, HHV of syngas and CGE was investigated. Raise in temperature improves the gasifier performance, it increases the production of CO and H_2 which leads to higher syngas yield, LHV and CGE. However, increasing ER lessens the production of CO and H_2 which results in reduction of gasification performance. The optimal values of CO and H_2 mole fraction and CGE of sawdust, wood chips and mixed paper wastes are located at 900˚C, 1000˚C and 1000˚C, respectively and ER range is between 0.20 - 0.35 regardless of the kind of biomass which is used as the feedstock. Among the three wastes considered, sawdust shows the highest CO mole fraction and LHV in the product syngas. Although, wood chips waste has the highest carbon percent among the other wastes, it has slight carbon yield, low CO mole fraction as well as lowest LHV. It is due to that it includes so high amount of moisture and moisture content indirectly effects on LHV of syngas, increasing moisture content strongly degrades the syngas LHV. Moreover, mixed paper waste shows the highest CGE (70.6%) at temperature of 1000˚C due to so high hydrogen content and the low HHV of its feedstock while for sawdust CGE is maximum around 65.8% and wood chips show lowest CGE (60%) among the three wastes.

Further works are required to evaluate the effects of moisture content on the gasification performance and to study the integrated gasifier with CHP to investigate the impact of operating parameters on power production.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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Paper V

Development of a new stoichiometric equilibrium-based model for wood chips and mixed paper wastes gasification by ASPEN Plus.
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DEVELOPMENT OF A NEW STOICHIOMETRIC EQUILIBRIUM-BASED MODEL FOR WOOD CHIPS AND MIXED PAPER WASTES GASIFICATION BY ASPEN PLUS

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ABSTRACT

Wood and paper residues are usually processed as wastes, but they can also be used to produce electrical and thermal energy through processes of thermochemical conversion of gasification. This study proposes a new steady state simulation model for down draft waste biomass gasification developed using the commercial software Aspen Plus for optimization of the gasifier performance. The model was validated by comparison with experimental data obtained from six different operation conditions. This model is used for analysis of gasification performance of wood chips and mixed paper wastes. The operating parameters of temperature and moisture content (MC) have been varied over wide range and their effect on the high heating value (HHV) of syngas and cold gas efficiency (CGE) were investigated. The results show that increasing the temperature improves the gasifier performance and it increases the production of CO and H_2 which leads to higher LHV and CGE. However, an increase in moisture content reduces gasifier performance and results in low CGE.

Keywords: waste biomass gasification, simulation model, Lower heating value, Cold gas efficiency

NOMENCLATURE

AFR	Air to fuel mass flow rate ratio, [kg_{air}/kg_{fuel}]
DCOALIGT	Density model for non-conventional components in ASPEN
CGE	Cold gas efficiency [%]
ER	Equivalence Ratio [%]
FC	Fixed carbon
Gp	Syngas yield, [m^3/kg fuel]
HCOALGEN	Enthalpy model for non-conventional components in ASPEN
HHV	Higher Heating Value, [J/m^3]
LHV	Lower Heating Value, [J/m^3]
MC	Moisture content [%]
MCINCPSD	Stream for non-conventional components in ASPEN, containing three substreams of MIXED, CIPSD and NCPSD class
R	Reaction
RE	Reactor
Sep	Separator
V	Volume, [Nm^3]
VM	Volatile matter
y	Mole fraction

1. INTRODUCTION

Increasing knowledge about the depletion of conventional energy sources and concern about environmental protection have encouraged the higher use of renewable energy alternatives [1]. Biomass as a renewable energy source, has obtained more interest because it is the only suitable and primary energy resource that can provide transportation fuels [2-4]. Biomass gasification is an attractive option that is getting huge attention for conversion of different feedstocks to energy. In gasification, waste like paper, cardboard, or wood is mixed with steam and oxygen at high temperature and is converted to syngas including mainly carbon monoxide and hydrogen. This gas is valuable in the chemical industry which can be used to produce solvents, plastics and fuels. Syngas can also be consumed directly as an energy source to generate power and hot water or steam.

Simulation of biomass gasification has been used to analyze the effect of various operating conditions on gasifier performance. The simulation can be performed using kinetic rate models or thermodynamic equilibrium methods. Thermodynamic equilibrium approaches are relatively simple and independent on gasifier design, which makes them more popular [5]. The thermodynamic equilibrium approaches are based on estimating the outlet compositions using different methods of stoichiometric and non-stoichiometric approaches. When implementing the stoichiometric method, a set of independent chemical reactions are specified, and the

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equilibrium concentrations are then calculated by solving for the extent of every reaction. However, when implementing the non-stoichiometric method, no reactions are specified and the concentrations of the gas species are evaluated to minimize the Gibbs energy of the products [5, 6]. Since the non-stoichiometric approach does not need a detailed specification of all the chemical reactions occurring in the reactor, numerous researchers have focused on this method. It is worth mentioning that the authors are only aware of very few published simulation studies on biomass gasification systems using the stoichiometric method [5]. Hence, the objective of this study is to develop a steady state computer model for waste biomass gasifier using ASPEN Plus simulator based on stoichiometric equilibrium method. Then this model is used to evaluate comparatively the gasification performance of two feedstocks of wood chips and mixed paper wastes. The effect of operating parameters of temperature and moisture content (MC) on high heating value (HHV) of produced syngas and cold gas efficiency (CGE) are investigated [7].

2. MATERIALS AND METHODS

A new kinetic free equilibrium model based on stoichiometric approach has been developed for the downdraft air gasifier of waste biomasses by using ASPEN Plus version 10. Penge Robinson equation of state with Boston-Mathias alpha function (PR-BM) was used to estimate all physical properties of the conventional components in the gasification process. This method can be appropriate for hydrocarbons and light gases as nonpolar/mildly polar mixtures and alpha parameter in this approach are temperature dependent variables that can be useful for the correlation of the vapor pressure of pure component when temperature is very high. Furthermore, HCOALGEN and DCOALIGT models were selected for enthalpy and density of biomass and ash which are non-conventional components. MCINCPSD stream comprising three substreams of MIXED, CIPSD and NCPSD class, was also used to define the structure of biomass and ash streams which are not available in Aspen Plus component database. Moreover, the model is based on the following 7 assumptions: (1) The model is at steady state, kinetic free and isothermal. (2) All gases are ideal gases, including hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), steam (H_2O), nitrogen (N_2) and methane (CH_4). (3) Char contains only carbon and ash in solid phase. (4) Tar and other heavy hydrocarbons are not considered. (5) Operation at atmospheric pressure (~ 1 bar). (6) No heat and pressure losses take place in the gasifier. (7) Simulation is based on stoichiometric equilibrium approach and based on reactions in Table 1 [7].

Figure 1 shows the flow chart of waste biomass gasification simulation using ASPEN Plus based on the stoichiometric approach and Table 2 is a brief description of the unit operations of the blocks used in the simulation. The BIOMSS stream was defined as a nonconventional stream and it was created by specifying the elemental and gross compositions of feedstock obtained from proximate and elemental analyses given in Table 3. In the next step, RYIELD, the yield reactor in ASPEN Plus, was brought to simulate the decomposition of the feed. In pyrolysis/decomposition step, the feedstock is converted to volatile materials (VM) and char. VM includes carbon, hydrogen, oxygen and nitrogen; Char is also converted into ash and carbon, by specifying the product distribution based on the proximate and ultimate analysis of the feedstock. The yield of volatiles is equal to the volatile content in the fuel according to the proximate analysis [8-10]. For stoichiometric equilibrium simulation of the combustion and gasification of biomass, REquil reactor was used in which homogeneous and heterogeneous reactions can be defined, simultaneously. However, due to the limitation of ASPEN Plus that each REquil can only contain one heterogeneous reaction, four REquil reactors (RE1-RE4) were considered for 4 heterogeneous reactions of R1, R2, R3, R5 (shown in Table 1).

TABLE 1: THE CONSIDERED REACTIONS IN THE MODEL

R1	$C+0.5O_2 \rightarrow CO$	Partial combustion
R2	$C+O_2 \rightarrow CO_2$	Complete combustion
R3	$C+H_2O \rightarrow CO+H_2$	Water-gas
R4	$H_2+0.5O_2 \rightarrow H_2O$	Hydrogen combustion
R5	$C+2H_2 \rightarrow CH_4$	Methanation

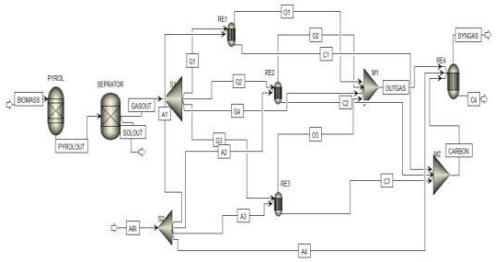

FIGURE 1: FLOW CHART OF WASTE BIOMASS GASIFICATION SIMULATION USING ASPEN PLUS

Two FSplit blocks were used for dividing streams of volatiles and air among reactors of RE1, RE2 and RE3 (for R1, R2 and R3). Then two Mixer blocks were used to mix outlet gasses and unburned carbons from the up and bottom of reactors, respectively; the product streams called OUTGAS and CARBON, respectively. Then, OUTGAS and CARBON streams with the rest of air stream were entered to RE4 for the heterogeneous reaction of R5 and homogenous reaction of R4. Eventually, the product gas called SYNGAS was exited from the up of RE4.

TABLE 2: DESCRIPTION OF ASPEN PLUS UNIT OPERATION BLOCKS USED IN MODEL

ASPEN Plus name	Block name	Description
Ryield	PYROL	Decomposition of non-conventional biomass to conventional components according to its proximate and ultimate analyses
Requil	RE1, RE2, RE3, RE4	Rigorous equilibrium reactor based on stoichiometric approach
Sep	SEPRATOR	Gas separation from ash by specifying split fractions
FSplit	S1, S2	Dividing of gas stream and air stream based on split fractions by S1 & S2, respectively
Mixer	M1, M2	Blending of gasses and carbons into one stream by M1 & M2, respectively

TABLE 3: ULTIMATE AND PROXIMATE ANALYSIS

Feedstocks	Wood chip	Mixed paper waste
Proximate analysis (wt%)		
Moisture	20	8.8
Volatile matter (VM)	80	84.2
Fixed carbon (FC)	18.84	7.5
Ash	1.16	8.3
Elemental analysis (wt%-dry basis)		
C	51.19	47.96
H	6.08	6.60
N	0.2	0.18
O	41.37	36.96

3. VALIDATION

For validating the presented model, the syngas composition obtained from ASPEN simulations were compared with the experimental results of Jayah et al [11]. In their work, rubber wood was used as feedstock in a down draft gasifier operated at atmospheric pressure and gasification temperature of 900 ˚C. Six different air to fuel mass flow rate ratios (AFRs) were considered and the comparisons of CO, H_2, CO_2 and N_2 concentrations are shown in Fig. 2. The deviation of the model results from experimental values is quantified by using statistical parameter RMS. RMS measures how much error there is between two data sets (experimental data and modeling values). Its value close to zero indicates lower error and more reliable model in prediction of results. The maximum RMS error of 1.89 is gained when six sets of experimental data are compared with the corresponding model values for syngas composition. The obtained RMS in this work is good and acceptable because it is not far from zero and also lower than other works in this field. For example Rupesh et al. [12] obtained RMS of 2.8 in comparison of experimental data and modeling values for product gas compositions.

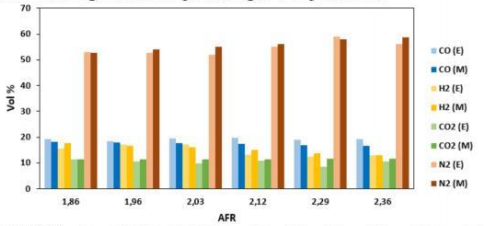

FIGURE 2: COMPARISON OF CO, H_2, CO_2 AND N_2 CONCENTRATIONS BETWEEN STOICHIOMETRIC MODEL (M) AND EXPERIMENTAL MEASUREMENTS (E)

4. RESULTS AND DISCUSSION

The developed model was used to study the gasification performance of two different waste feedstocks of wood chips and mixed paper waste. Then, the effect of gasifier temperature and MC on LHV of produced gas and CGE has been investigated. The LHV of syngas is calculated as [8, 13]:

$$LHV_{syngas}\left(\frac{kj}{Nm^3}\right) = 4.2\times(30\times y_{CO} + 25.7\times y_{H_2} + 85.4\times y_{CH_4}) \quad (1)$$

where y is the mole fraction of gas pieces in the syngas (dry basis).

The CGE is also calculated by using equation (2) [8, 14]:

$$CGE(\%) = \frac{G_P \times LHV_{syngas}}{HHV_{fuel}} \times 100 \quad (2)$$

where G_P is the syngas yield that is the volume of total product gas from the gasification per unit weight of fuel in normal conditions (Nm^3 kg fuel-1). HHV_{fuel} is the higher heating value of fuel (MJ kg fuel-1) [15].

$$HHV_{fuel}\left(\frac{Mj}{kg}\right) = 0.312\times(FC) + 0.1534\times(VM) \quad (3)$$

According to equation (3), heating value is a function of weight fractions of fixed carbon and volatile matter in the dry and ash-free conditions.

4.1 Effect of temperature and MC on LHV

The effect of gasifier temperature on LHV of syngas for two feedstocks was examined in the window of 500-1500 ˚C, while all the remaining operating conditions were fixed (equivalence ration (ER)=0.4 and MC according to Table 3). As shown in Fig. 3, the increase in temperature results in an increase in the LHV of the syngas until a specific temperature that is called optimum temperature. At very low temperature of 500 ˚C the existing carbon in the biomass is not used completely, so the

syngas would be produced at a low yield. At such a low temperature, unburned carbon and methane will remain in the syngas. By increasing the temperature more carbon is oxidized and converted to carbon monoxide in accordance with partial combustion reaction (R1). Methane is also transferred into hydrogen by reverse methanation reaction (R5). At higher temperature, water gas reaction (R3) shifts toward the production of both carbon monoxide and hydrogen. Hence, increasing the gasifier temperature favors hydrogen and carbon monoxide production, which leads to the improvement of heating value of syngas (based on equation (1)). However, at a specific temperature, the yield of H_2 and CO approach a plateau; the onset of this plateau is typically the optimal gasifier temperature for every type of waste stream evaluated here. The optimum operating temperature of the down draft gasifier for wood chips and paper wastes are both around 900 ˚C. LHV values for wood chips and mixed paper wastes at optimum temperatures are about 3.79 and 4.06 MJ Nm^3, respectively.

Wood chips shows lower heating value than paper waste due to relatively lower dry basis mole fraction of CO and hydrogen in the syngas. The production of CO and hydrogen is dependent on the biomass composition and it is clear from the composition of feedstock streams provided in Table 3 that although wood chips have highest percentage of carbon, they include a high amount of moisture. MC indirectly effects on LHV of syngas (Fig. 4). Increasing moisture content strongly degrades the syngas LHV. Because of much higher moisture content in the fuel, the percentage of carbon and hydrogen in wet basis decrease then leads to lower production of carbon monoxide and hydrogen in the syngas.

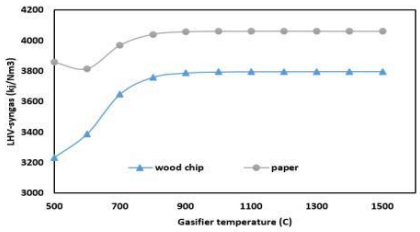

FIGURE 3: EFFECT OF TEMPERATURE ON LHV

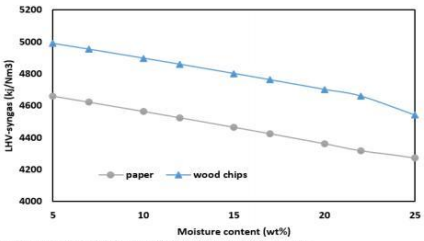

FIGURE 4: EFFECT OF MC ON LHV

4.2 Effect of temperature and MC on CGE

In our model temperature has been varied from 500-1500˚C and the corresponding CGE as the most crucial parameter for economic efficiency evaluation of the gasifier is calculated. The results have been depicted in Fig. 5. Accordance to equation (2), CGE is dependent on different parameters of syngas yield, HHV of fuel and LHV of syngas. Syngas yield and LHV depend on the amount of carbon monoxide, hydrogen and methane in the product syngas and HHV of wood chips and paper wastes were calculated 18.37 and 16.63 MJ kg^{-1}, respectively. Mixed paper waste shows highest CGE (70.5%) at temperature of 900 ˚C while for wood chips CGE is maximum around 60%. Fig. 6 shows that increasing MC reduces the value of CGE, stemming from the reduction of LHV (Fig. 4). For the two waste biomass streams, the amount of CGE is under 65% as long as ER is more than 15%. It follows that MC should be kept below this level.

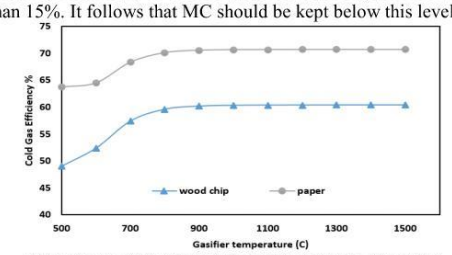

FIGURE 5: EFFECT OF TEMPERATURE ON CGE

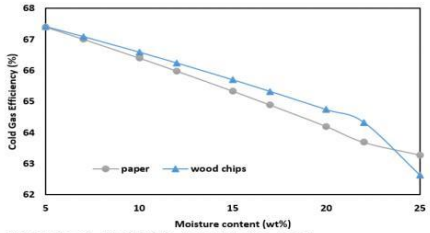

FIGURE 6: EFFECT OF MC ON CGE

5. CONCLUSION

A new steady state model simulating downdraft waste biomass gasification was developed using Aspen Plus based on stoichiometric equilibrium approach, modified with restricted chemical reactions equilibrium in the gasification reduction zone. The model was successfully validated with experimental data of downdraft rubber wood gasification, with good agreement on the main syngas compositions. Subsequently the effect of gasification temperature and biomass moisture content on HHV of syngas and CGE was investigated. Increasing temperature improves the gasifier performance, it increases the production of CO and H_2 which leads to higher LHV and CGE. However, high moisture content reduces gasifier performance and results in low CGE. In order to achieve optimal gasification performance, it was recommended that the gasification

temperature should be around 800-1000 °C and the biomass moisture content should be less than 15%.

ACKNOWLEDGEMENTS

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Paper VI

Performance analysis and environmental assessment of small-scale waste biomass gasification integrated CHP in Iceland.
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Performance analysis and environmental assessment of small-scale waste biomass gasification integrated CHP in Iceland

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ABSTRACT

Integrated waste biomass gasification with cogeneration heat and power (CHP) is an attractive method for high efficiency electricity generation. It not only involves wastes as fuel but also helps in reduction of releasing pollutant gasses to the atmosphere. In this research, a simulation model is developed to assess performance and environmental impacts of producing electricity from gasifying of organic wastes in Iceland: garden, timber/wood, and paper mixed wastes. The objectives are to find the optimal operating conditions to make the highest electrical efficiency and the evaluation of global warming (GWP), acidification (AP) and eutrophication (EP) potentials in regard to the environmental impact of the system. Moreover, the environmental assessment for the integrated waste gasification and CHP is compared with waste incineration in a conventional and currently running system. Our results show that the electricity production from waste gasification technology appears to be more environmentally friendly than waste direct combustion in all impact categories considered. Among the systems, timber and wood waste is the most beneficial from performance and environmental perspectives. The 1 kW h electricity production from timber through gasification would lead to a GWP of 0.07 kg CO_2eq, AP of 0.09 kg SO_2eq, and EP potential of 0.36 kg NO_3eq.

1. Introduction

Globally, a major method under consideration to meet the energy demand is to explore and exploit new sources of energy that are renewable and environmentally friendly. Renewable energy sources like solar, wind, hydro wave, geothermal and biomass offer attractive prospects due to their abundance and zero/low cost [1–4]. Among the wide variety of energy options, biomass has obtained more interest. Unlike fossil fuels that take many years to be replenished, biomass can be regenerated relatively quickly. Also, when it burns, carbon dioxide releases back in to the atmosphere, but this biogenic CO_2 is not counted as a contributor to global warming [5–8]. Among different kinds of biomass fuels, energy crops, crop residues and organic wastes are the most important alternatives, of which, the last group has received much attention as a potentially large option of renewable energy [7].

Currently, biomass gasification integrated combined heat and power (CHP) or only power production plants have been introduced as efficient and environmentally friendly methods for extracting energy from different sources of organic wastes. In gasification, waste like wood, paper or cardboard is mixed with steam and air/oxygen at high temperature and is converted to syngas consisting mainly of carbon monoxide and hydrogen. This gas can then be consumed directly as an energy source to generate power and hot water/steam through the CHP process [9,10].

Various research mention that gasification is an emerging but promising technology, especially in comparison with commercially available technologies like incineration [11–14]. Gasification plants also produce much lower levels of air pollutants. The process also reduces the environmental impact of waste disposal because it utilizes waste as a feedstock and uses less water than traditional coal based power plants. Additionally, the by-products of gasification are non-hazardous and readily marketable. Equally important, waste gasification can be implemented as a more reliable energy supply technology for cities or towns that are far from the central energy networks and need to have a district heat and power system.

In this paper, we will explore the potential of gasification for energy production and organic waste treatment for small communities in Iceland. Most of Iceland municipalities, which are semi-

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autonomous administrative zones, contain several disparate towns/cities with a population lower than 10 thousand settlements [7]. In these very distant regions where a wide grid is not feasible, decentralized power generation by gasification offers a viable option for meeting the electricity needs of the local population.

An overview of different Icelandic municipalities is shown in Fig. 1. West (A), Suðurnes (B), South (C), Capital area (D), East (E), Northeast (F), Eyjafjörður (G), Northwest (H) and Westfjords (I), [15]. Western Iceland consists of 10 municipalities with a total of 15 thousand occupants in 2010. Suðurnes contains 5 municipalities with a total of 21 thousand inhabitants in 2010. The Capital Area covers 8 municipalities with 200 thousand residents. Southern Iceland consists of 14 municipalities with a total of 23 thousand inhabitants. East contains 9 municipalities with a total of 12 thousand inhabitants. Northeast covers 6 municipalities with a total of 5 thousand occupants. Eyjafjörður includes 8 municipalities with 24 thousand residents. There are 8 municipalities in Northwest with a total population of 7500 and finally Westfjords contains 9 municipalities with 7 thousand inhabitants in 2010 [15].

Organic waste from households, industry and services is a valuable source for biofuels production in Iceland. The Icelandic Environmental Agency set up a National plan to reduce the amount of organic wastes that are landfilled or incinerated over the years. A general estimation shows that approximately 60% of the total waste is organic material of which 70% is obtained from industry and services and 30% is from the household sector [15]. The main categories of organic waste that can be fed to a gasifier are garden waste, timber and wood waste, and mixed paper waste. Fig. 2 shows the total amount of these kinds of organic waste for various Icelandic parts in 2020. As is shown in Fig. 2, the Capital area is the dominant region in all waste production with more than 60% of the Iceland population in this area. However, the Capital area occupies just 1% of total area. This is because of the lack of development and urbanization in this location, lack/shortage of proper climate and geographical conditions in other places and transportation issues [7].

The primary objective of this research is to analyze the performance of the biomass gasification integrated CHP based on the simulation model developed by using ASPEN Plus. The case study assesses power production in Iceland from 1ton of 3 different Icelandic organic wastes: garden waste, timber and wood waste, and paper mixed waste. Then, as a sensitivity analysis, we examine the effect of operating parameters like temperature and equivalence ratio (ER) to know where the overall system is optimal to reach the maximum electrical efficiency. An environmental assessment of the considered system for the 3 mentioned wastes at optimal conditions is also studied in this paper. Finally, the estimations of global warming, acidification and eutrophication potentials for the integrated system of gasification and CHP are compared with waste incineration in a conventional and currently running system in Iceland.

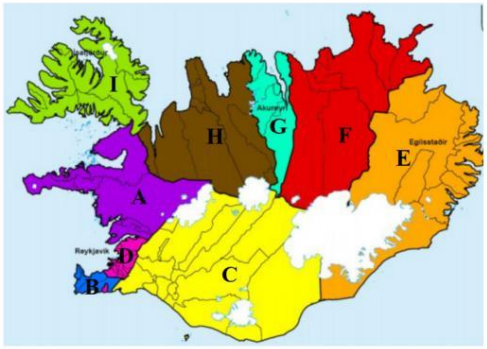

Fig. 1. Overview of Icelandic municipalities [15].

2. Material and methods

2.1. System description

The system considered by this work includes all the process steps from the initial resources to the end products (Fig. 3).

In the resource step, garden, timber and wood, and paper mixed wastes are the main input resources. Energy and water are also considered as accessory inputs. Diesel fuel used by trucks for transportation and electricity consumed for driving force and heat generation in process units are also considered. The electricity production in Iceland is derived from geothermal and hydropower making the main source of clean energy. Waste is transferred from the waste fields to pre-processing units that are located next to gasification and power production plants. The gasification process consists of drying, pyrolysis, combustion and gasification [16]. Drying occurs at a temperature of 100–150 °C. Generally, the moisture in biomass ranges from 5% to 35% but it is reduced to lower than 5% during drying. The moisture content can be lessened by using several technologies, like natural drying, mechanical drying, and thermal drying. Natural drying by air is the easiest way for water reduction in the fresh biomass. In this way, the achievable moisture content depends on the temperature and air relative humidity. Compressible biomass, can be dried by mechanical dewatering. Mechanical presses include centrifuges, screw, belt filter, ring, drum, and roller presses. The major drawback of these kind of drying is their energy consumption and maintenance costs. If the drying process is located close to the conversion plant, waste heat can be used for drying. Wet biomass can either be directly dried by hot air, steam, or flue gas in belt conveyers, fluidized beds, spray dryers, or indirectly by heat-transfer via a casing, in a drum. The selection of the drying process depends on the properties of the biomass, such as size, morphology, and heat sensitivity, as well as the requirements of the entire process chain [17–19].

Pyrolysis takes place in the range of 200–700 °C, and in this step the volatile components in the biomass are vaporized as it is heated in the absence of oxygen. The volatile vapor is a mixture of hydrogen, carbon monoxide, carbon dioxide, methane, hydrocarbon gases, tar and water vapor. Finally, combustion occurs at 700–1500 °C and gasification in the range of 800–1100 °C. At this stage, oxygen supplied to the gasifier reacts with the combustible substances, resulting in CO_2 and H_2O, which subsequently undergo reduction upon contact with the char produced from pyrolysis. Reduction yields combustible gases like hydrogen, carbon monoxide and methane through a series of reactions [20]. The produced syngas next enters a combustion chamber followed by a gas turbine. The combination of these two modules represents the behavior of a combustion engine where the reaction with air occurs. The thermal content of the gas is obtained as the heat of combustion is removed and used to convert boiler feed water to high pressure steam. The generated steam finally drives a steam turbine, producing additional power. Key assumptions regarding inputs for each process are listed in Table 1 [5–8].

2.2. Simulation model

A kinetic free equilibrium model has been developed for a

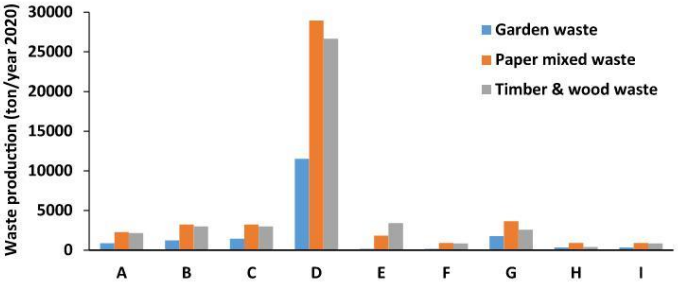

Fig. 2. Waste production for different Icelandic municipalities in 2020 [15].

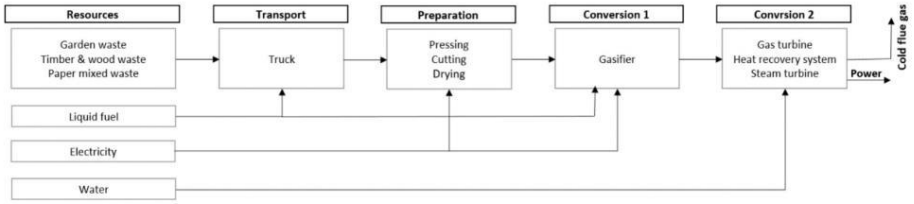

Fig. 3. System boundaries, considered technologies and associated inputs (energy and material).

Table 1
List of some assumption regarding inputs for each step [5–8].

Step	Unit	Amount	Comment
Resources			
Waste input	ton	1	
Transport			
Distance	km	100	Distance from fields to energy conversion plants
Diesel fuel	L/km.ton	0,06	
Preparation			
Electricity for pressing & cutting	kWh/ton	5,48	
Conversion 1			
Unit Fuel oil	L/ton	0,2	It is for start-up of the gasifier
Unit Electricity	kWh/ton	83	
Conversion 2			
Isentropic efficiency of compressor	%	90	
Mechanical efficiency of compressor	%	99	
Isentropic efficiency of gas turbine	%	90	
Isentropic efficiency of steam turbine	%	92	

downdraft air gasifier of waste biomass using ASPEN Plus version 10. The Penge Robinson equation of state with the Boston-Mathias alpha function (PR-BM) was used to estimate all physical properties of the conventional components in the gasification process. Furthermore, HCOALGEN and DCOALIGT models were selected for the enthalpy and density of the biomass and ash which are non-conventional components. MCINCPSD stream comprising three substreams of MIXED, CIPSD and NCPSD class, was also used to define the structure of the biomass and ash streams which are not available in the Aspen Plus component database.

Fig. 4 shows the flow chart of the waste biomass gasification simulation using ASPEN Plus. The BIOMSS stream was defined as a nonconventional stream and it was created by specifying the elemental and gross compositions of feedstock obtained from proximate and elemental analyses given in Table 2 [21,22]. Drying occurs at 150 °C achieving the reduction of moisture to 5 wt% of the original sample. This step is directed by the stoichiometric reactor RSTOIC in Aspen Plus. This particular module is used to perform chemical reactions of known stoichiometry [23]. The key operation for this step is performed by writing a FORTRAN statement in the calculator block. RSTOIC converts a part of feed to form water which requires the extent of reaction known as [1]:

$$Feed \rightarrow 0.0555084 H_2O$$

In this step, the moisture of each feedstock is partially evaporated and then separated using a separator model, (model id: SEP1). After being stripped from moisture, RYIELD, the yield reactor is used to simulate the decomposition of the feed. In the pyrolysis step, the feedstock is converted to volatile materials (VM) and char. VM includes carbon, hydrogen, oxygen and nitrogen; Char is also converted into ash and carbon, by specifying the product distribution based on the proximate and ultimate analysis of the feedstock [9]. Then RGibbs is used to simulate gasification of the

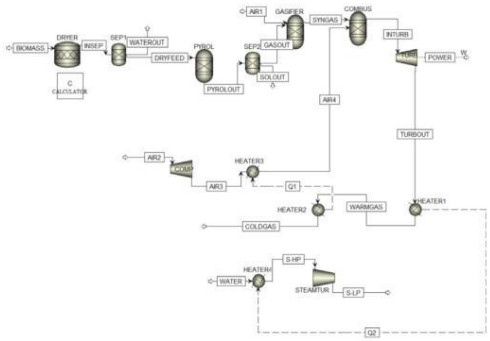

Fig. 4. Flow chart of gasification simulation in Aspen Plus.

biomass. The reactor calculates the syngas composition by minimizing the Gibbs free energy and assumes complete chemical equilibrium. The decomposed feed and air enter the RGibbs reactor where partial oxidation and gasification reactions occur. Another RGibbs reactor is also used in the combustion section with minimum air mixing. Principally, this process is also based on minimization of the Gibbs free energy. The combustion chamber is followed by a gas turbine [24]. The thermal content of the gas, obtained as the heat of combustion is removed and used to convert water to high pressure steam though a HEATER. The generated steam finally drives a steam turbine and produces additional power [25]. The solid lines in Fig. 4 stand for the mass streams, whereas the dashed lines are for the heat streams. The system is assumed to be auto-thermal so that a part of the biomass is combusted inside the gasifier in order to provide the heat required in situ. Heat is also provided by the hot product gas, as well as the combustion chamber, and is utilized wherever needed.

2.3. Environmental assessment

Environmental assessment can be defined as identifying and estimating of the environmental impacts of existing and proposed systems to mitigate the relevant negative effects prior to making decisions [26]. The impact categories in this paper are global warming (GWP), acidification (AP) and eutrophication (EP) potentials. GWP concentrates on greenhouse gas emissions (GHG) and their impact on global warming. GHGs are atmospheric gas compounds (CO_2, CH_4 and NO_2) that trap heat through emitting radiation in the atmosphere. The increase in the amount of these gases results in keeping the surface of the earth warmer by absorption of the sun light that passes through the atmosphere freely [5,26]. Acidification is also an environmental problem caused by acidified rivers/streams and soil due to anthropogenic air pollutants of SO_2, NH_3, H_2SO_4, H_2S, HCL, SO_3 and NO_x. These kind of emissions come down to the ground as acid rain or snow to be absorbed into lakes, rivers, and soil. As a result, surface water, ground water and soil are acidified in ways that cause devastation of forests and many shelled animals. Eutrophication is also a phenomenon in which inland waters are heavily loaded with excess nutrients due to chemical fertilizers or discharged wastewater, triggering rapid algal growth and red tides. The major substances with impacts on eutrophication were found to be NO_x, NH_3, N_2, and NO_3 in the case of air [27].

The impact assessment methods employed in this work are based on IPCC 2007 and other research works in this field [8,28]. The GWP, AP and EP factors for key input in to the system and their factors for different emitted substances are summarized in Table 3 [6–8] and Table 4 [29], respectively.

3. Results and discussion

3.1. Performance analysis

In this study, the developed model for waste biomass gasification has been used to investigate the gasification performance of three feedstocks in Iceland: garden, timber and wood, and paper mixed wastes. The goal is to find the optimal operating conditions in order to produce the highest power efficiency. The important operating variables that affect power performance are the gasifier temperature and the equivalence ratio (ER). The effect of temperature and ER on power efficiency of the gasifier system is shown in Fig. 5 and Fig. 6, respectively. The power efficiency is the index of the power generated from the system compared to the original energy contained in the biomass feed and is defined by [23]:

$$\eta_{power} = \frac{W_{gas\ turbine} + W_{steam\ turbine} - W_{compressor}}{M_{biomass} \times LHV_{biomass}} \quad (1)$$

The sensitivity results in Figs. 5 and 6 are studied at standard conditions of 1 ton input of feedstock, a 2.5 air to biomass ratio and a gasifier temperature in the window of 500–1500 °C. As seen in Fig. 5, all wastes show a similar increasing behavior as the temperature rises. At a very low temperature of 500 °C, the existing carbon in the biomass is not used completely, so the syngas production would not be at a good rate. Unburned carbon and methane will remain in the syngas, while by increasing the temperature

Table 2
Ultimate and proximate analysis of feedstocks [21,22].

	Garden waste	Timber & wood waste	Paper mixed waste
Proximate analysis			
Proximate analysis (wt%)			
Moisture	50	5.01	10.24
Volatile matter (VM)	84.5	93.06	84.60
Fixed carbon (FC)	14.5	6.38	9.40
Ash	1	0.56	6
Ultimate analysis			
Elemental analysis (wt%- dry basis)			
C	50.12	56,8	43,41
H	6.40	7,28	5,82
N	0.14	0,18	0,25
Cl	0	0,82	0
S	0.08	0,07	0,2
O	42.26	34,29	44,32

Table 3
GWP, AP and EP factors for different inputs [6–8].

Input	Unit	GWP factor ($kgCO_{2eq}$/unit)	AP factor (gSO_{2eq}/unit)	EP factor (gNO_{3eq}/unit)
Electricity generated from geothermal	kWh	0.058	1.95	2.8
Transport by truck	ton.km	0.3	2.1	4.2
Liquid fuel used in gasifier	lit	2.76	10.5	21

Table 4
GWP, AP and EP factors for different emitted substances [29].

	GWP factor ($kgCO_{2eq}$/$kg_{substance}$)	AP factor ($kgSO_{2eq}$/$kg_{substance}$)	EP factor ($kgNO_{3eq}$/$kg_{substance}$)
CO_2	1		
CH_4	25		
N_2			0.042
O_2			
S			
SO_2		1	
NH_3		1.88	3.64
NO		1.07	0.02
N_2O	298		
CL_2			
HCL		0.88	
NO_2		0.7	0.013
H_2SO_4		0.65	
NO_3			1

more carbon is oxidized and converted to carbon monoxide. Methane is also transformed into hydrogen by a reverse methanation reaction. Hence, increasing the gasifier temperature favors hydrogen and carbon monoxide production, leading to high LHV syngas enter to the combustion chamber and resulting high temperature gases entering the turbine. Raising the turbine inlet temperature increases output power from the gas turbine, as well as the steam turbine, because more steam is produced through the heat recovery from the high temperature flue gas. However, at a specific range of temperature, power efficiency increases in a gradual way such that this span can be the optimum gasifier temperature for each waste. The optimum operating temperature of the down draft gasifier for the three studied wastes was 900–1000 °C.

Moreover, Fig. 5 shows timber and wood waste has dominant statues for power efficiency among the three wastes due to relatively higher net power production through the system. The amount of power production is dependent on the biomass composition and it is clear from the composition of feedstocks provided in Table 2 shows timber and wood has the highest percentage of carbon and hydrogen and lowest amount of moisture. Hence, this kind of waste would be the best option to be fed to a gasifier and power production plant. However, garden waste with the highest moisture content of 50% has the lowest potential for power production. Moisture content indirectly effects output power as a higher moisture content in the fuel leads to a decrease in the percentage of carbon and hydrogen in a wet basis leading to a lower production of carbon monoxide and hydrogen as well as lower LHV.

Air equivalence ratio (ER) is the ratio of the air entering in the system to the stoichiometric demanded for air which constitutes a significant factor for consideration. At low ER, biomass reactions will approach pyrolysis, whereas at a high ER the excess amount of oxygen oxidizes the fuel completely and causes biomass combustion; then the syngas production and consequently power generation decline. Hence, it is important to find the appropriate range of ER for biomass gasification. In this case, the ER in the gasifier was varied from 0.2 to 0.65 and its influence on the power efficiency are shown in Fig. 6 for the three wastes. As shown in Fig. 6 the optimum ER lies between 0.2 and 0.3, 0.4–0.5 and 0.35–0.45 for timber and wood, paper mixed and garden wastes, respectively. At optimum span of ER, the power efficiency from gasification of timber and wood waste is higher than that of paper mixed and garden wastes averaging 42% and 63%, respectively.

3.2. Environmental assessment

The environmental impact assessment of the integrated

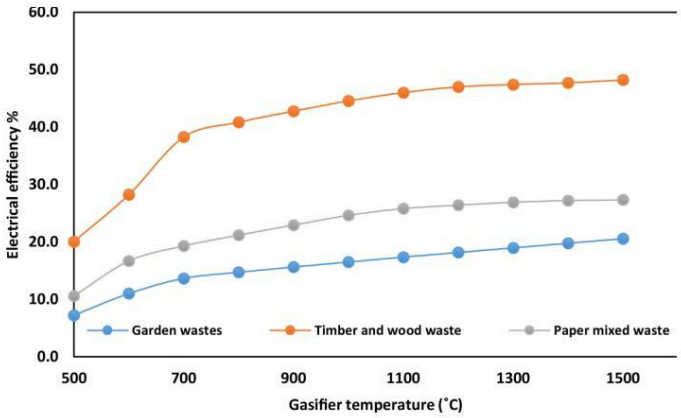

Fig. 5. Effect of temperature on power efficiency.

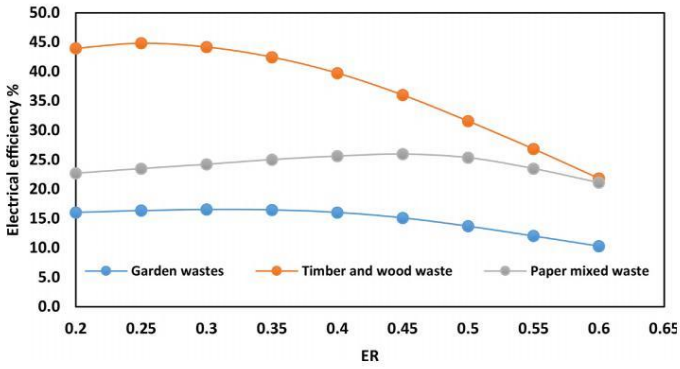

Fig. 6. Effect of ER on power efficiency.

gasification CHP system is analyzed with the three categories of global warming, acidification and eutrophication potentials. This assessment is directed based on a functional unit of 1 ton of input feedstock and under the optimum operating conditions obtained in section 3.1 for each waste. Discussion in relation to each impact category is presented in the following.

3.2.1. Global warming potential

The GWP comparison of CHP gasification for the studied wastes with direct combustion of them and their GWP contributions through the gasifying are shown in Fig. 7 and Fig. 8, respectively. Garden waste with GWP of 56 $kgCO_{2eq}$ per ton has the highest GHG emissions. This is due to garden waste having the highest moisture content (50%) and requiring more energy for drying leading to higher GHG emissions releasing to the atmosphere. The largest contribution for all wastes is made by transport through consumption of diesel fuel following with cutting, handling and drying in preparation process. Of the process chain, conversion 2 including the combustion chamber, gas and steam turbines makes up the smallest share of GWP contributions because when biomass is burnt, carbon dioxide releases back to the atmosphere but this biogenic CO_2 is not counted as a contributor to global warming. As seen in Fig. 7, on a per ton of raw feedstock basis, the degree of reduction in global warming if gasification is used instead of direct combustion is around 90%. Obviously, the production of electricity from waste based on gasification technology appears to be more environmentally friendly than waste direct combustion if GWP is evaluated. This is because gasification technology has a lower level of exhaust emissions of significant air pollutants and a higher amount of carbon retained in the ash.

3.2.2. Acidification potential

The comparison of electricity production from waste relying on gasification versus direct combustion in relation to acidification potential impact is presented in Fig. 9. Regarding this index, the production of electricity from garden, timber and paper wastes gasification create 16, 54 and 12 $kgSO_{2eq}$ per ton of raw feedstock, respectively. The emissions of acidic gases from the combustion process in the conversion 2 sector accounts for a major share of the impact, leaving a relatively minor share to the other processes. As seen in Fig. 9, CHP gasification of timber and wood waste has the worst AP impact. This is because the highest amount of acidic gasses like NO, NO_2, SO_2 and HCL are released to the atmosphere. However, it is still much more environmentally friendly in comparison to direct combustion.

3.2.3. Eutrophication potential

In Fig. 10, the eutrophication impact is compared for CHP gasification of three different wastes versus wastes combusted directly. Production of electricity from consumption of 1 ton of garden, timber and wood wastes in gasification releases 98, 225 and 141 $kgNO_{3eq}$, respectively. The most important contribution to this impact is made by the emissions of particulate matters, N_2, NO_3, NO and NH_3 from the combustion process, whereas the contribution made by the other processes, preparation, transport and gasification is relatively minor.

To have a more accurate comparison of different feedstocks, the environmental impacts per kWh electricity produced in the three studied waste-gasification process is displayed in Fig. 11. As seen in Figs. 5, 6 and 11, timber and wood waste is the most beneficial from the performance and environmental perspectives. At various temperatures and equivalence ratios, the system based on timber and wood waste has the highest statues in electrical efficiency, as well as lowest levels of in pollutant gas emissions among the other systems. This can be explained by the fact that this kind of waste contains high level of carbon and hydrogen which leads to high power production and also includes a fair amount of moisture which causes it to require lower energy for drying in the preparation sector leading to slight GHG emissions releasing to the atmosphere.

4. Conclusions

According to the assessment results, three main points of conclusion can be drawn as indicated below:

1) Simulation results indicated that optimal operating conditions for producing the highest power efficiency are gasifier temperatures of 900–1000 °C for all waste and an equivalence ratio between 0.2 and 0.3, 0.4–0.5 and 0.35–0.45 for timber and wood, paper mixed and garden wastes, respectively. At the optimum range of temperature and ER, the power efficiency from gasification is 45, 26 and 16% for timber and wood, paper mixed and garden wastes, respectively.
2) The production of electricity from waste gasification integrated with CHP appears to be more environmentally friendly than waste incineration in all impact categories considered. This can be explained by the fact that gasification technology has a lower

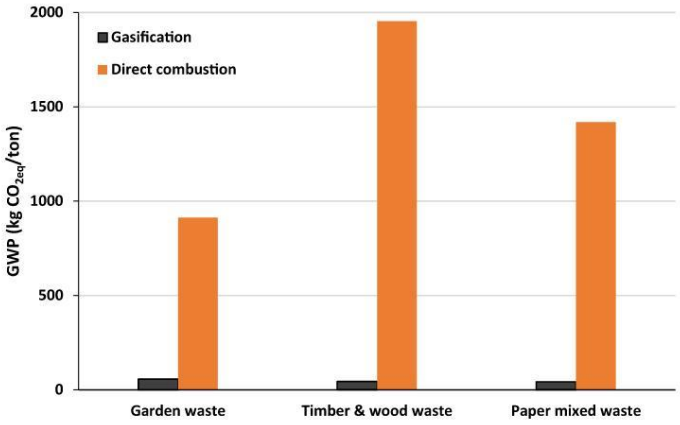

Fig. 7. GWP of waste gasification for electricity production versus waste direct combustion.

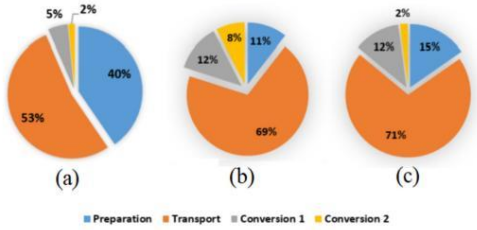

Fig. 8. GWP contributions for 3 wastes gasification: (a), garden (b), timber & wood (c), paper mixed.

level of exhaust emissions of significant air pollutants and a higher amount of carbon retained in the ash.

3) Among the systems, timber and wood waste is the most beneficial from the performance and environmental perspectives. The production of 1 kW h of electricity from timber through gasification would lead to a GWP of 0.07 kg CO_2eq, AP of 0.09 kg SO_2eq, and EP potential of 0.36 kg NO_3eq. Of the processes in the chain, the largest contribution for all wastes is made by transport through consumption of diesel fuel following by cutting, handling and drying in the preparation process. Whereas conversion 2 containing the combustion chamber, gas and steam turbines occupies the smallest share in environmental contributions.

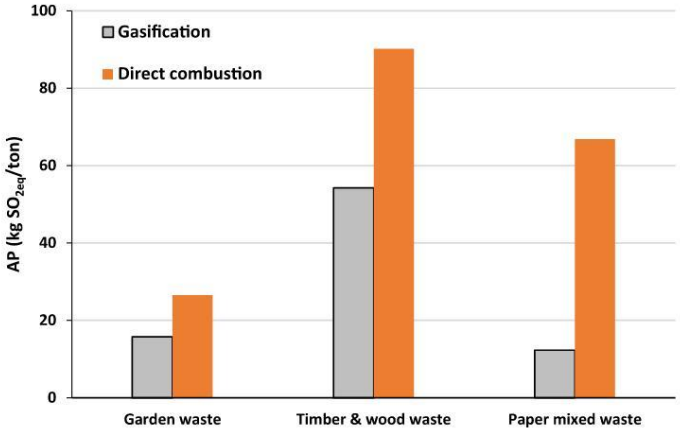

Fig. 9. AP of waste gasification for electricity production versus waste direct combustion.

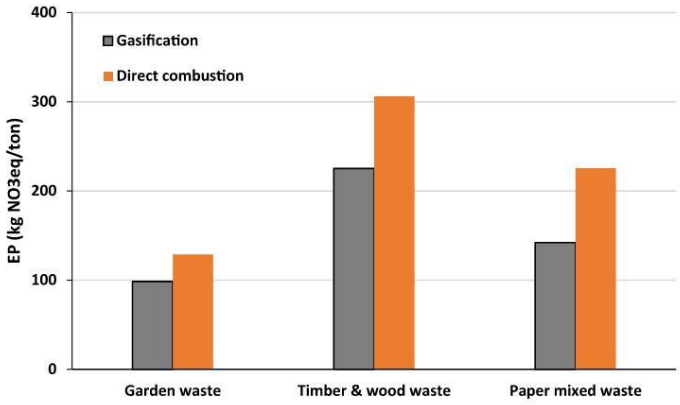

Fig. 10. EP of waste gasification for electricity production versus waste direct combustion.

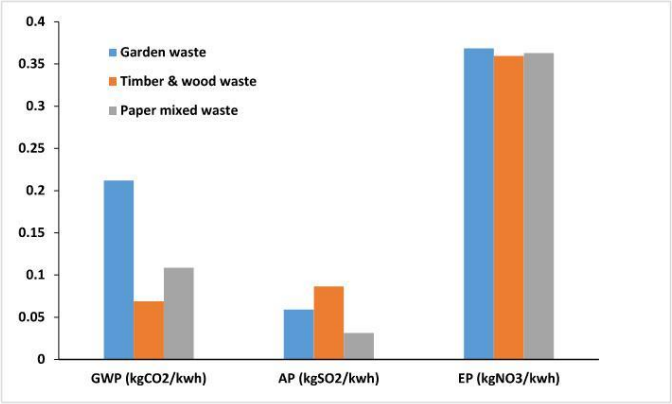

Fig. 11. GWP, AP and EP of waste gasification per 1 kW h net power production.

Declaration of competing interest

The authors declare no conflicts of interest.

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Paper VII

Simulation of small-scale waste biomass gasification integrated power production: a comparative performance analysis for timber and wood waste.
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Simulation of small-scale waste biomass gasification integrated power production: a comparative performance analysis for timber and wood waste

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ABSTRACT

A simulation model for integrated waste biomass gasification with cogeneration heat and power has been developed using Aspen Plus. The model can be used as a predictive tool for optimization of the gasifier performance. The system has been modeled in four stages. Firstly, moisture content of biomass is reduced. Secondly biomass is decomposed into its elements by specifying yield distribution. Then gasification reactions have been modeled using Gibbs free energy minimization approach. Finally, power is generated through the internal combustion engine as well as heat recovery system generator. In simulation study, the operating parameters like temperature, equivalence ratio (ER) and biomass moisture content are varied over wide range and their effect on syngas composition, low heating value (LHV) and electrical efficiency (EE) are investigated. Overally, increasing temperature and decreasing ER and MC lead to improvement of the gasification performance. However, for maximum electrical efficiency, it is important to find the optimal values of operating conditions. The optimum temperature, ER and MC of the down draft gasifier for timber and wood waste are 800˚C, 0.2-0.3 and 5%. At such optimum conditions, CO and H_2 reach to the highest production and LHV and EE are around 7.064 MJ Nm^{-3} and 45%, respectively.

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1. INTRODUCTION

The finite nature of conventional fossil fuels, increasing concerns due to environmental impact and health and safety considerations are encouraging to find renewable energy sources and alternative technologies to produce power [1, 2]. In the last decades the interest in biomass has increased due to the growing attention to sustainable energy. Unlike fossil fuels that take so many years to be refilled, biomass can be regenerated relatively quickly and when it burns, carbon dioxide releases back to the atmosphere but this biogenic CO_2 is not counted as a contributor to global warming [3-6].

Currently, biomass gasification integrated power production unit has been introduced as an efficient and environmentally friendly way for extracting energy from different organic wastes. Biomass gasification is a process of converting biomass fuel into syngas as a mixture of combustible gases through a sequence of thermo-chemical reactions. The produced gas through the biomass gasification can be conditioned to burn

cleanly, like natural gas. This means a customer can install a gasifier system in an existing facility and reuse much of the same boiler, dryer, and ducting equipment [7-9].

Much important, waste gasification can be implemented as a more reliable energy supply technology for places which are far from the central energy networks and require district heat and power systems. Most of Iceland municipalities also contain several disparate towns/cities with the population lower than 10 thousand settlements [5]. Hence, in this paper, we study the potential of gasification for energy production for small communities in Iceland. Organic waste produced from household, industry and service sectors is an available option for biofuels production in Iceland. A general estimation shows that approximately 60% of the total waste is organic material which 43, 41 and 16% of that are paper mixed, timber and wood and garden wastes [10]. Safarian et. al. [11] found that among the various Icelandic waste biomass gasification systems, timber and wood waste is the most beneficial from the performance and environmental perspectives. The production of 1 kWh electricity from timber through the gasification would lead to a global warming potential of 0.07 kg CO_{2eq}, acidification potential of 0.09 kg SO_{2eq}, and eutrophication potential of 0.36 kg NO_{3eq}.

The primary aim of this work is to develop a steady state computer model for performance analysis of waste biomass gasifier integrated with CHP using Aspen Plus. The case study is in Iceland to assess power production from 1 ton of timber and wood waste as approximately most existing and greatest environmental beneficial biomass feed stock in this country. Finally, the effect of operating parameters like temperature, equivalence ratio (ER) and biomass moisture content (MC) on syngas composition, low heating value (LHV) and electrical efficiency (EE) are investigated to find the optimum conditions making highest LHV and electrical efficiency.

2. MATERIAL AND METHODS

An equilibrium simulation model has been developed for waste biomasses gasification integrated with CHP by using Aspen Plus. Penge Robinson equation of state with Boston-Mathias alpha function (PR-BM) was applied to calculate physical properties of the conventional components in the gasification process. HCOALGEN and DCOALIGT models were also employed for enthalpy and density of biomass and ash which are non-conventional components. MCINCPSD stream comprising three substreams of MIXED, CIPSD and NCPSD class, was also considered to define the biomass structure and ash streams which are not available in Aspen Plus component database [7]. The flow chart of the system simulated by using Aspen Plus is shown in Figure 1. The BIOMSS stream was defined as a nonconventional stream and it was created by specifying the elemental and gross compositions of feedstock obtained from proximate and elemental analyses given in Table 1 [11].

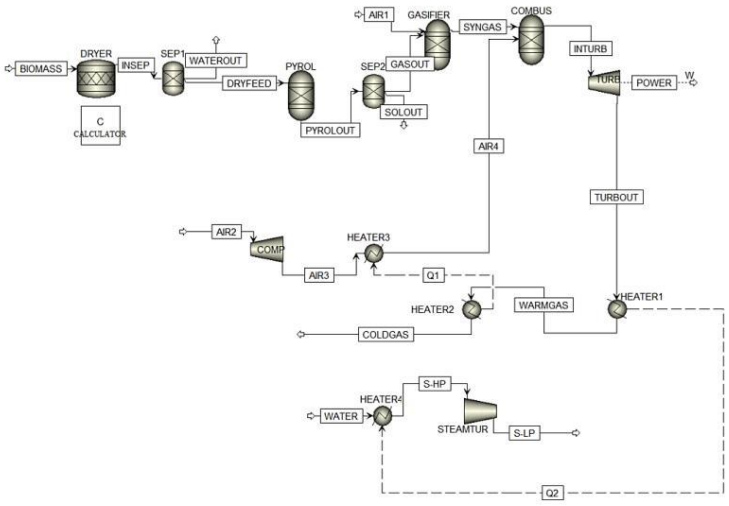

Figure 1. Flow chart of gasification simulation in Aspen Plus

Table 1. Ultimate and proximate analysis of timber & wood waste [11]

Proximate analysis	
Proximate analysis (wt%)	
Moisture	5.01
Volatile matter (VM)	93.06
Fixed carbon (FC)	6.38
Ash	0.56
Ultimate analysis	
Elemental analysis (wt%- dry basis)	
C	56.8
H	7.28
N	0.18
Cl	0.82
S	0.07
O	34.29

Drying occurs at 100°C to achieve the moisture reduction to 5 wt.% of the original sample. This step is directed by the stoichiometric reactor RSTOIC in the Aspen Plus. This particular module is used to perform chemical reactions of known stoichiometry [12]. After drying, RYIELD, the yield reactor is brought to simulate the feed pyrolysis. In this step, the feedstock is converted to volatile materials (VM) and char. VM contains carbon, hydrogen, oxygen and nitrogen; Char is also converted into ash and carbon, by specifying the product distribution based on the proximate and ultimate analysis of the feedstock [7]. Then RGibbs is used to simulate the biomass gasification. The reactor calculates the syngas composition by minimizing the Gibbs free energy and assumes complete chemical equilibrium. The decomposed feed and air enter to the RGibbs reactor where partial oxidation and gasification reactions occur. Another RGibbs reactor is also simulated for combustion section with minimum air mixing. Principally, this process is also based on minimization of Gibbs free energy. The combustion chamber is followed by a gas turbine [13, 14]. The thermal content of the gas, obtained as the combustion heat is removed and consumed to convert water to high pressure steam though a HEATER. The generated steam finally drives a steam turbine and produces additional power [15, 16]. The solid lines in the Figure 1 stand for the mass streams whereas the dashed lines are for the heat streams. The system is assumed to be auto-thermal so that a part of the biomass is combusted inside the gasifier in order to provide the heat required in situ. Heat is also provided by the hot product gas as well as the combustion chamber and utilized wherever needed.

3. RESULTS AND DISCUSSION

The developed model for waste biomass gasification is used to investigate the gasification performance of timber and wood waste. The effect of gasifier temperature, equivalence ration (ER) and moisture content (MC) on syngas composition, lower heating value (LHV) of produced gas and electrical efficiency (EE) are investigated. The lower heating value of product gas is calculated as [17, 18]:

$$LHV_{syngas}(kj/Nm^3) = 4.2\times(30\times y_{CO} + 25.7\times y_{H_2} + 85.4\times y_{CH_4}) \quad (1)$$

where y is the mole fraction of gass pecies in the syngas (dry basis).

The main goal is finding optimal operating conditions to make the highest electrical efficiency. The electrical efficiency is the index of the power generated from the system compared to the original energy contained in the biomass feed and is defined by [12]:

$$\eta_{electrical} = \frac{W_{gas\ turbine} + W_{steam\ turbine} - W_{compressor}}{M_{biomass}\times LHV_{biomass}} \quad (2)$$

3.1. Effect of temperature on system performance

The effect of gasifier temperature on syngas mole fractions produced through the timber and wood waste gasification, is shown in Figure 2. Figure 3 also shows the LHV of syngas and the electrical efficiency of the gasifier system as a function of temperature. The sensitivity results in Figures 2 and 3 are studied at standard conditions of 1-ton input biomass, 0.25 air equivalence ratio and gasifier temperature in the window of 500-1500˚C.

Based on Figure 2, the present carbon in the timber and wood waste is not used completely at low temperature (500˚C), so the syngas production could not be in an acceptable rate. At such a low temperature,

methane and unburned carbon will stand in syngas while by increasing temperature more carbon is oxidized and converted to carbon monoxide based on partial combustion reaction. Methane is also transferred into hydrogen by reverse methanation reaction. Water gas reaction also goes toward the production of both CO and H_2 at high temperature. Hence, increasing the gasifier temperature favors hydrogen and carbon monoxide production, leads to the improvement of heating value of syngas as shown in Figure 3. However, at a specific temperature, yield of H_2 and CO reach to an approximately constant values that this point is called the optimum gasifier temperature. The optimum operating temperature of the down draft gasifier for timber and wood waste is 800˚C. Methane production also decreases sharply at temperatures above 600˚C. LHV value for timber and wood waste at optimum temperature is about 7.054 Mj Nm^{-3}. Improving LHV of syngas leads to entering gases at high temperature to the gas turbine. Raising the turbine inlet temperature ameliorates output power from that as well as the steam turbine. It is because of that more steam is produced through the heat recovery from the hot flue gas. Electrical efficiency also increases in a gradual way near the optimum temperature, it reaches about 45% around 800˚C.

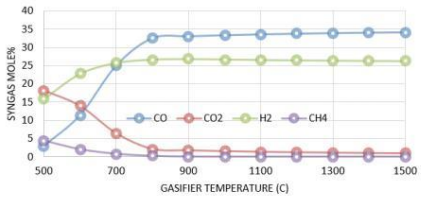

Figure 2. Effect of temperature on syngas mole fraction (dry basis, ER: 0.25)

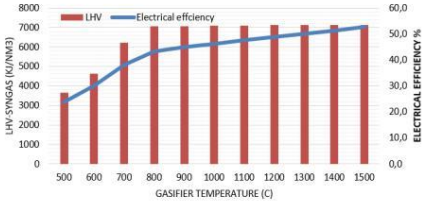

Figure 3. Effect of temperature on syngas LHV and electrical efficiency (ER: 0.25)

3.2. Effect of ER on system performance

Equivalence ratio (ER) as the ratio of the actual air value supplied to the gasifier to the stoichiometric air is a significant factor for showing the role of oxidizing agent. At low ER, biomass reactions will approach to the pyrolysis, however at higher values of ER the excess amount of oxygen is combusted which leads to the declining of syngas production. Hence, it is important to find the appropriate range of ER for biomass gasification that is investigated in our work. For timber and wood waste gasification, ER is varied from 0.2-0.65 and its influence on the syngas compositions is shown in Figure 4. The H_2 and CO mole fractions decrease with increasing ER but an opposite trend for CO_2 is exhibited. This is due to when ER rises, more oxygen is supplied for biomass reactions, so fuel goes toward the full combustion. The optimum ER lies between 0.2-0.3, till mole fractions of CO and H_2 are higher than 25%. By increasing ER, the heating value of the syngas and electrical efficiency also decrease as shown in Figure 5. As a whole, the LHV of the product gas and electrical efficiency depend strongly on ER and ER is function of syngas compositions in (1). At optimum span of ER, LHV and electrical efficiency from timber and wood waste gasification are around 7.064 MJ Nm^{-3} and 45%.

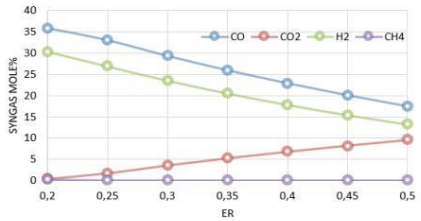

Figure 4. Effect of ER on syngas mole fraction (dry basis and gasifier temperature is 900˚C)

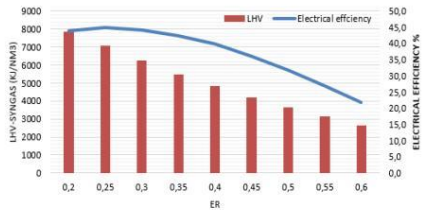

Figure 5. Effect of ER on syngas LHV and electrical efficiency (gasifier temperature is 900˚C)

3.3. Effect of MC on system performance

The moisture content of the biomass is varied from 5 to 35% to investigate its effect on the performance of the gasifier integrated with CHP. Figure 6 shows the effect of biomass moisture content on syngas compositions. Moreover, impact of MC on syngas LHV and electrical efficiency of the system is depicted on Figure 7. Moisture content has a remarkable effect on gasifier performance. It is known that a high MC content is responsible for the reduction of H_2 and CO in the produced gas and for the increase in CO_2 mole fraction. As a consequence, the heating value of the syngas decreases while the MC increases. According to equilibrium mathematical method for downdraft gasifiers, the increase in biomass MC of 35% results in the reduction of the LHV of the syngas by about 1.8 MJ Nm^{-3}. Increasing moisture content also strongly degrades the system electrical efficiency. The increase in biomass MC of 35% results in the declining of the electrical efficiency by 32%.

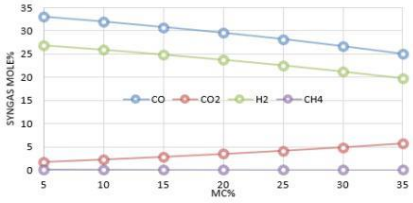

Figure 6. Effect of MC on syngas mole fraction (dry basis, gasifier temperature: 900˚C and ER: 0.25)

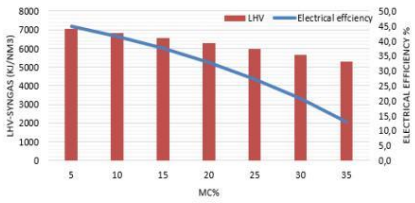

Figure 7. Effect of MC on syngas LHV and electrical efficiency (gasifier temperature: 900 ˚C and ER: 0.25)

4. CONCLUSION

A steady state equilibrium-based model was developed for waste biomass gasification using Aspen Plus simulator. The model was used for comparative analysis of the gasification performance of timber and wood waste in Iceland. In the model, sensitivity analysis was performed and the impact of varying gasifier temperature, ER and MC on syngas composition, LHV of syngas and electrical efficiency was investigated. Raise in temperature improves the gasifier performance, it increases the production of CO and H_2 which leads to higher LHV and electrical efficiency. However, Increasing ER degrades the CO and H_2 production which results in reduction of gasification performance. Moisture content has also a significant effect on gasifier performance. A high MC content is responsible for the reduction of H_2 and CO in the product gas. Consequently, the increase in biomass MC of 35% results in the reduction of the LHV of the syngas and the system electrical efficiency by about 1.8 MJ Nm^{-3} and 32%, respectively. The highest values of CO and H_2 mole fraction, LHV and EE of the gasification system-based timber and wood waste located at 800˚C, 0.20-0.3 of ER and 5% of MC. In these conditions, LHV and electrical efficiency are around 7.064 MJ Nm^{-3} and 45%, respectively.

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Paper VIII

Techno-Economic and Environmental Assessment of Power Supply Chain by Using Waste Biomass Gasification in Iceland.
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ORIGINAL PAPER

Techno-Economic and Environmental Assessment of Power Supply Chain by Using Waste Biomass Gasification in Iceland

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Abstract
In this paper, technical, economic and environmental assessments are carried out for power supply chain by using timber and wood waste (T&WW) gasification in Iceland. The Icelandic municipalities were clustered into 35 subgroups based on various number of households/ inhabitants. Different expenses were taken into consideration, like capital, installation engineering, operation and maintenance costs and the interest rate of the investment. Regarding revenues, they come from the electricity sale and the fee paid by the Icelandic municipalities for waste collection and disposal. The economic feasibility was conducted based on the economic indicators of net present value (NPV) and discounted payback period (DPP), bringing together three different scenarios, with interest rates of 8% for Scenario 1, 10% for Scenario 2 and 13% for Scenario 3. The environmental analysis was also performed relied on the environmental impacts of global warming (GWP), acidification (AP) and eutrophication (EP) potentials. The results show that changing the interest rate does not have significant impact on NPV and DPP for all studied scenarios. NPV is positive for the municipalities with more than 150 inhabitants or for a gasification plant with the capability to generate greater than 45 kW. Moreover, electricity generation based on T&WW gasification would lead to a GWP of 13 tonCO_{2eq} (Subgroup 1) to 469 tonCO_{2eq} (Subgroup 35), AP of 173.6 tonSO_{2eq} (Subgroup 1) to 6187.2 tonSO_{2eq} (Subgroup 35) and EP potential of 331.9 tonNO_{3eq} (Subgroup 1) to 11,827.7 tonNO_{3eq} (Subgroup 35), yearly.

Keywords Waste biomass gasification · Techno-economic analysis · Environmental assessment · Power supply chain · Waste to energy

Introduction

Waste is a major problem that causes not only serious economic losses, but also significant environmental impacts. Better living standards, tourist streams and economic growth accelerate the waste generation in Iceland. Improper management of wastes has led to increased public concerns about health and environmental impacts. The total amount of municipal solid waste (MSW) in Iceland in 2010 has been estimated to 76 ± 6 thousand ton, based on data available from Sorpa, the waste management company in the Capital area. In other words, the annual amount of MSW per capita has been estimated to 222–257 kg (Sundberg et al. 2010). The amount of MSW produced in 2030 is estimated to approximately 100 ± 7 thousand ton. Generally 60% of this amount is organic material which 43, 41 and 16% of that are paper mixed, timber and wood and garden wastes, respectively (Safarian et al. 2020b; Sundberg et al. 2010).

Landfilling and incineration have been the only methods of disposal of solid wastes in Iceland, while most landfill sites have been open dumping areas, which pose serious environmental and social threats. An incinerator in Skutulsfjörður caused carcinogenic and toxic chemicals to be found in meat and milk (Halldorsson et al. 2010). Soil and incinerator-emissions measurements at several sites, including Kirkjubaejarklaustur, reveal emissions 85 times above the EU limit (Niðurstöður úr mælingum á díoxínum í jarðvegi 2011). These problems resulted in the shuttering of several incinerators and the withdrawal of Icelandic meat and milk products (Halldorsson et al. 2010; Safarian and Unnthorsson 2018).

All these problems demonstrated the need to find more responsible alternatives than conventional incineration and landfilling (Mohapatra 2013; Omari et al. 2014). The method

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must be environmentally friendly, low cost and energy efficient and must reduce land use and emissions. These advantages are all found in modern gasification technology. Gasification is an attractive alternative that has recently gained considerable attention, as it disposes of solid waste without landfilling or incineration problems (Brunner et al. 2004; Porteous 2005).

Unlike the relatively uncontrolled combustion occurring in incineration, gasification is a partial oxidation at elevated temperature (600–1700 °C) that converts organic components to a Synthesis Gas (syngas), consisting mainly of CO, H_2, small amount of CH_4, minor quantities of different hydrocarbons (tars), inorganic impurities (H_2S, HCl, NH_3, HCN, HF, alkalis) and particulates (Ofori-Boateng et al. 2013; Safarian et al. 2019d; Samadi et al. 2019). Air, O2, steam, CO_2 or a mixture of all these can be used as an agent in the gasifier. Air gasification produces a syngas with small lower heating value (LHV) among 4–6 MJ/Nm^3, while oxygen gasification produces a syngas with a medium LHV in the range of 10–20 MJ/Nm^3 (Leckner 2015).

Beneficially, MSW gasification can be applied for small/medium scales that leads to dramatic reduction of some pollutants emission as furans, dioxins, and NO*x* and the possibility of the utilization of the syngas in high efficiency thermal devices like internal combustion engine and gas turbines (Luz et al. 2015). Hence, waste gasification can be installed as a reliable energy supply technology for places which are far from the central energy networks and require district heat and power systems (Safarian et al. 2019a, 2019c, 2020c).

In this paper, we will explore the potential of timber and wood waste (T&WW) gasification for energy production in small communities in Iceland (T&WW is the most existing biomass feedstock in this country). In this way, a comprehensive techno-economic and environmental assessment of T&WW gasification facilities integrated with electricity generation unit will be directed to propose a sustainable waste to power system adapted with conditions in Iceland.

Material and methods

Case study description

Iceland is one of the biggest islands in Europe, 103,000 m^2 in area. The population of Iceland is only about 300,000 (2.9 per m^2). Iceland is therefore one of the most sparsely populated countries in the world. The entire country is divided into regional municipalities that have self-determination and responsibility regarding their own affairs. More than 60% of the population lives in the capital city area. There are 72 municipalities in Iceland that their population varies from 43 inhabitants in the smallest ones, to more than 126,000 in the biggest. About 55% of Icelandic municipalities have lower than 1000 residents and 70% of them occupies lower than 2000 populations. In these kinds of regions where wide grid is not feasible, small-scale gasification integrated with power generation offers a viable option for meeting the electricity needs of the local population (Safarian and Unnthorsson 2018).

In order to have a wide evaluation of the economic feasibility of the installation of gasification facilities for all disparate Icelandic zones, we established 35 subgroups based on various number of households/inhabitants (Table 1). In each subgroup, the study was conducted over hypothetical cases, according to the number of households as each household includes 5 persons.

Organic waste produced from industries, household and services sectors is a valuable source for biofuels production in Iceland. In this way, the Icelandic Environment Agency sets up a national plan to decrease the amount of organic wastes which are landfilled or incinerated for years. The main categories of organic waste that can be used as input feedstock into gasifier are timber and wood waste, garden waste, and paper mixed waste. Safarian et al. (2019a, b, c, d) (Safarian et al. 2019c) showed that among the different gasification systems based on various wastes in Iceland, timber and wood waste is the most beneficial from the performance and availability perspectives.

Timber waste is generally defined as unpainted and painted timber and is produced from construction/demolition work, packaging waste and pallets. The total amount of timber waste in Iceland in 2010 has been estimated to

Table 1 The considered subgroups with the number of household and population

Subgroups	Household	Persons	Subgroups	Household	Persons
1	10	50	19	190	950
2	20	100	20	200	1000
3	30	150	21	210	1050
4	40	200	22	220	1100
5	50	250	23	230	1150
6	60	300	24	240	1200
7	70	350	25	250	1250
8	80	400	26	260	1300
9	90	450	27	270	1350
10	100	500	28	280	1400
11	110	550	29	290	1450
12	120	600	30	300	1500
13	130	650	31	310	1550
14	140	700	32	320	1600
15	150	750	33	330	1650
16	160	800	34	340	1700
17	170	850	35	350	1750
18	180	900			

around 37 ± 11 thousand ton and it has been projected to reach approximately 49 ± 15 thousand ton in 2030. Wood waste is also available from forestry, and it has been estimated to nearly 8260 ton/year. Totally, timber and wood waste mainly consist of softwood, with a composition of 45% cellulose, 22% hemicellulose and 28% lignin as well as extractives, acids, salts and minerals. Hence, all produced T&WW can be considered as potential for syngas production (Sundberg et al. 2010).

Process Description

The studied system in this paper includes all the process steps from resources to the end product (Fig. 1).

Timber and wood waste is the significant resource entering to the system, and liquid fuel and electricity are also the accessory inputs. The proximate and elemental analyses of T&WW are shown in Table 2.

Diesel fuel is used in trucks for transportation, and electricity is applied for driving force and heat generation over the process. The electricity production in Iceland is derived from geothermal and hydropower that makes Iceland's main source of clean energy. T&WW is transferred from the waste fields to pretreatment part that is next to gasification and electricity generation unit. The gasification process consists of drying, pyrolysis, combustion and gasification (Safarianbana et al. 2019). Drying occurs at a temperature 100–150 °C. Typically, the moisture in biomass is among 5–35% that it is reduced to lower 5% during drying. Pyrolysis occurs in the range of 200–700 °C; in this step, biomass is heated in the absence of oxygen then its volatile components are vaporized. The volatile vapour consists mainly of H_2, CO, CO_2, CH_4, hydrocarbon gases, tar and steam. Finally, combustion turns up in 700–1500 °C and gasification occurs between 800 and 1100 °C. In this work, the down draft reactors are considered that operate at atmospheric pressure, to gasify T&WW and air is used as the gasification agent, resulting in CO_2 and H_2O, which subsequently undergo reduction upon contact with the char produced from pyrolysis. Reduction yields combustible gases as H_2, CO, and CH_4 through a series of reactions (Safarian et al. 2019d). Then the produced syngas enters in internal combustion engine that is modelled as a combustion chamber followed by a gas turbine. The combination of these two modules represents the behaviour of a combustion engine where the reaction with air occurs (Safarian and Bararzadeh 2012; Safarian et al. 2013). The input values and key assumptions are shown in Table 3, we also used from our waste biomass gasification simulation model developed by ASPEN Plus (Safarian et al. 2020a) to have the main values of the downdraft gasifier characteristics, operational parameters and the flue gas composition which are listed in Table 3.

Table 2 Ultimate and proximate analyses of timber and wood waste (Freeman et al.)

Parameters	Value (%)
Proximate analysis (wt%)	
Moisture	5.01
Volatile matter (VM)	93.06
Fixed carbon (FC)	6.38
Ash	0.56
Ultimate analysis (wt%—dry basis)	
C	56.8
H	7.28
N	0.18
Cl	0.82
S	0.07
O	34.29

Techno-Economic Assessment

All prices are expressed in K€ (kilo-euro). In the economic assessment, three scenarios are considered based on different interest rates: 8% in Scenario 1, 10% in Scenario 2 and 13% in Scenario 3. A computer program has been developed to investigate these scenarios for all subgroups shown in Table 1. The model is able to evaluate the economic performance of each one. Cash flow analysis, total cost, Net Present Value (NPV) and Discounted Payback Period (DPP) are standardized financial indicators to assess the profitability of projects. A project is an economically attractive while it has the lowest DPP and the NPV higher than zero. NPV

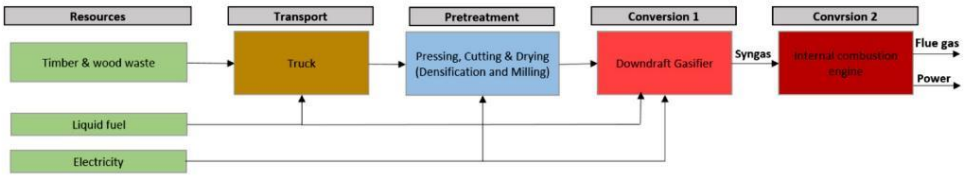

Fig. 1 System boundaries, technologies, energy and material streams

Table 3 Input values, assumptions, gasifier characteristics, operational parameters and flue gas composition

Step	Unit	Amount	Comment
Transport			
Distance	km	100	Distance from fields to energy conversion plants
Diesel fuel	L/km. $ton_{T\&WW}$	0.06	
Preparation			
Electricity for pressing & cutting	kWh/ $ton_{T\&WW}$	5.48	
Conversion 1			
Type of gasifier			Downdraft fixed bed (autothermal)
Gasification agent			air
Gasification pressure	kPa	101.3	
Gasification temperature	°C	800	
Equivalence Ratio (ER)	–	0.25	
Specific air mass flow rate consumption	$kg/kg_{T\&WW}$	108	
Unit Fuel oil consumption	L/ $ton_{T\&WW}$	0.2	It is for start-up of the gasifier. $ton_{T\&WW}$ refers to amount of T&WW that enters to gasifier after pre-process step
Unit Electricity consumption	$kWh/ton_{T\&WW}$	83	$ton_{T\&WW}$ refers to amount of T&WW that enters to gasifier after pre-process step
Conversion 2			
Isentropic efficiency of compressor	%	90	
Mechanical efficiency of compressor	%	99	
Net produced power	kWh/yr	2820.8 MT&WW (kg/hr) + 2293.3	as functional of mass flow rate of biomass
Specific mass flow rate of flue gas exited from gas turbine	$kg/kg_{T\&WW}$		
CO		0.226	
CO2		1.62	
H2		0.00247	
H2O		0.645	
CH4		0	
N2		5.316	
O2		0.082	
S		0	
SO2		0.0013	
H2S		0	
NH3		0	
NO		0.049	
N2O		0	
CL2		0	
HCL		0	
NO2		0.000037	
H2SO4		0	
NO3		0	

is the difference between the present value of cash inflows and the present value of cash outflows over a period of time and it is calculated based on Eq. (1) (Safarian et al. 2014):

$$NPV = \sum_{n=1}^{t} \frac{CF_n}{(1+r)^n} - C_c \quad (1)$$

where CF_n is the annual cash flow, being the difference between Revenues (R) and Expenditures (E); Operation and Maintenance Costs ($C_{O\&M}$),r is the discount rate (8%, 10% and 13% for Scenarios 1, 2 and 3, respectively); $_{Cc}$ is the total capital costs of investment and is the lifetime of the investment (15 years). DPP gives the number of years to break even from undertaking the initial expenditure, by

discounting future cash flows and recognizing the time value of money and it is calculated according to Eq. (2):

$$DPP = \frac{LN(\frac{1}{1-\frac{C_{CXF}}{CF}})}{LN(1+r)}. \quad (2)$$

The periodic cash flow, with all the revenues and expenditures, is calculated by considering the incomes from the generated electricity, and the credits for the Waste Treatment Bill (WTB) (Luz et al. 2015). The expenditures also include the $_{Cc}$ and $C_{O\&M}$. C_c is divided into three categories: hardware price ($_{Cg}$), installation cost (25% of C_g) and engineering costs, the engineering costs includes engineering and design (13% of C_g), purchasing & construction (14% of C_g), fuel handling/preparation (9% of C_g) and electrical/balance of plant (6% of C_g) (Porcu et al. 2019; Sara et al. 2016). C_g is the overall price of gasifier system on the basis of various capacities. In this work, we considered 0.75, 1.5, 2, 5, 10, 20, 50, 100, 200, 300, 400 and 500 kW for the small-scale existing gasifiers capacities and extracted their prices from various companies (Fig. 2) (Chongqing Fengyu Electric Co. 2019; GreenVinci Biomass Energy Co. 2019; Labs 2019; Qingdao Kexin New Energy Technology.Co. 2019; Shandong Rotex Machinery. 2019; Tiger Machinery Group Co. 2019).

The whole yearly $C_{O\&M}$ can be determined by the sum of the costs for the maintenance cost (2% of $_{Cc}$), insurance and tax (2% of $_{Cc}$), waste disposal (15% of $_{Cc}$), electricity cost, liquid fuel cost and personnel cost. Electricity costs are calculated based on electricity consumers and liquid fuel costs are estimated for fuel consumers with 7000 h/year of plant availability (Porcu et al. 2019; Sara et al. 2016). The unitary cost of electrical and fuel energies supplied in Iceland are equal to 0.03 $/kWh and 1.08 $/lit (0.91 €/$ as conversion rate) (Safarian and Unnthorsson 2018). Personnel cost includes annual labour, cost. A total of two employees were assumed for plant operation management (1 person/shift and 2 shifts/day), with a yearly cost of 60,000 €/year per person in Iceland.

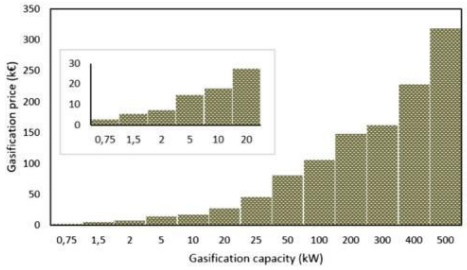

Fig. 2 Gasifier prices for different capacities

In relation to revenues, the selling price of electricity to normal households and small businesses in Iceland is about 124.69 $/MWh (Orkusetur 2019). Hence, the sale price of the generated electricity based on waste gasification was considered at 109.89 $/MWh (100 €/MWh) in our work. Moreover, The Icelandic municipalities pay a fee (WTB) by weight, to the private companies, for the collection and disposal the MSW in sanitary landfills. The WTB for collection and disposal of the MSW varies from 90–170 €/ton through over Iceland. The highest amout is related to Vestmannaeyjar, an archipelago off Iceland's south coast with 111 km distance from Reykjavik (the Capital of Iceland). All produced waste in Vestmannaeyjar need to be collected and transferred to other Icelandic municipalities for disposal. Hence, WTB for this area is in the top due to geographical conditions and expensive transportation. In this work, a mean value of 130 €/ton is used.

Environmental Assessment

Assessment of the environmental impacts of projects involves evaluating and providing information on the probable effects of specific undertakings on the environment. The environmental indicators studied in this work are global warming (GWP), acidification (AP) and eutrophication (EP) potentials. GWP concentrates on greenhouse gas emissions (GHG) including CO_2, CH_4 and NO_2 that trap heat through emitting radiation in the atmosphere (Safarian et al. 2018, 2019b). Acidification is also an environmental problem caused by acidified streams and soil due to anthropogenic air pollutants of SO_2, NH_3, H_2SO_4, H_2S, HCL, SO_3 and NO_x. The main substances with eutrophication impacts are also NO_x, NH_3, N_2, and NO_3 in the case of air. The environmental assessment methods applied in this paper are based on IPCC 2007 and other research works in this field (Nguyen et al. 2013; Paengjuntuek et al. 2015). The GWP, AP and EP factors for key input to the system are summarized in Table 4 (Nguyen et al. 2013; Safarian and Unnthorsson 2018).

Results and Discussion

Technical Performance

The calculations performed in this paper show that it is beneficial technically and energetically to produce electrical power from the waste biomass downdraft gasification integrated with power generation. Whether this technology can be successfully applied for the purpose of electricity distribution in small municipalities geographically isolated depends on economic and environmental considerations.

Table 4 GWP, AP and EP factors for different inputs (Nguyen et al. 2013; Safarian and Unnthorsson 2018)

Input	Unit	GWP factor ($kgCO_{2eq}$/unit)	AP factor (gSO_{2eq}/unit)	EP factor (gNO_{3eq}/unit)
Electricity generated by geothermal	kWh	0.058	1.95	2.8
Transport by truck	ton.km	0.3	2.1	4.2
Liquid fuel used in gasifier	lit	2.76	10.5	21

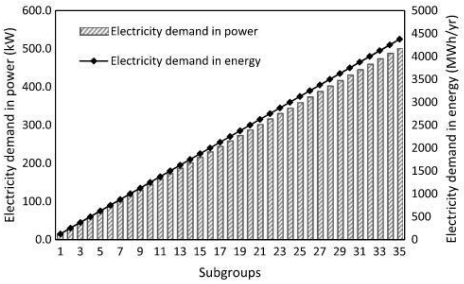

Fig. 3 Electrical energy and power demand for each subgroup

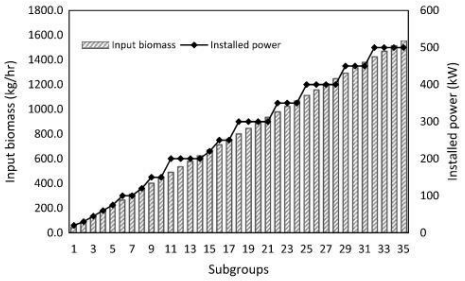

Fig. 4 Input T&WW and installed power for subgroups

The yearly electricity consumption per capita in the household sector in Iceland is around 2.5 MWh per capita. Based on these data, Iceland occupies the fourth place in electricity consumption in the world (Norway, Sweden and Finland have the first, second and third statues, respectively) (explained 2019). By using these data, the yearly electricity consumption and power demand for each subgroup are calculated and shown in Fig. 3. Obviously, as the population grows, energy demand also increases. Power demand varies form 14.3 kW for the first subgroup with 50 persons (10 households) to 499,4 kW for the last one with 1750 persons (350 households).

By considering the demanded power for each subgroup and existing gasifiers capacities (Sect. 2.3), the required gasifiers capacities which need to be installed for each case have been extracted and depicted in Fig. 4. As a constraint, more than two gasifiers have not been taking in account for each subgroup. For example, one gasifier with 20 kW capacity has been selected to satisfy 14.3 kW as the requested power for the first subgroup. However, for the second subgroup, two gasifiers with 5 and 25 kW need to be installed to supply 28.5 kW demanded. Analysing the subgroups 9 and 10 shows that, it is possible that both have the same installed power (150 kW), equally two gasifiers with 100 and 50 kW were considered for both with the requested power of 128,4 and 142,7 kW, respectively. The same happens for the cases of 6 and 7 (100 kW), 11 to 14 (200 kW), 16 and 17 (250 kW), 18 to 21 (300 kW), 22 to 24 (350 kW), 25 to 28 (400 kW), 29 to 31 (450 kW) and 32 to 35 (500 kW).

Figure 4 also shows the relation between the installed power and the amount of T&WW that is fed to the system for treatment and power production. Clearly, the installed power does not increase in the same proportion as that of the input waste, due to different capacities used for each system. For some cases, the installed gasification capacities are oversized, so the required investments of the capital costs and O&M costs need to be considered depending on the size of the components.

Economic Assessment

Costs and Revenues

The total cost of the generation plant for each population subgroup for the basic scenario (scenario 1) is shown together with the corresponding installed power in Fig. 5. The total cost varies from about 1100 k€ (Subgroup 1) to more than 2000 k€ (Subgroup 35). The total cost increases as the installed power grows, this trend is kept till up 5, but subgroups 6 and 7 present relatively lower cost in comparison to the former subgroup. It can be explained that the requested power of these subgroups (100 kW) are met only by using one gasifier. This is also similar for the subgroups of 11–14 (200 kW), 18–21 (300 kW), 25–28 (400 kW) and 32–35 (500 kW).

Percentage shares depicted in Fig. 6 are contributions of hardware, installation, engineering and annual O&M costs in total cost for basic scenario. The yearly O&M costs occupy

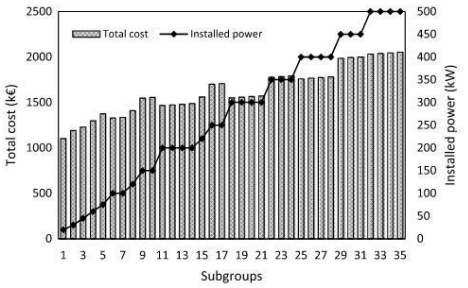

Fig. 5 Total costs on the basis of the installed power for scenario 1

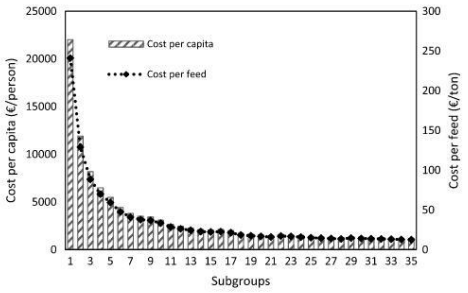

Fig. 7 Specific cost of T&WW gasification per input waste and per capita

more than 70% of total cost for the first subgroup, it has also the dominant statue among different kinds of costs for subgroups 1–8. However, the highest share is related to gasification system price for subgroups 9–35.

Figure 7 presents the specific cost for the implantation of new facilities for power production by using T&WW gasification, per ton of waste treated. It has been pointed out that the specific cost per ton of T&WW is inversely proportional to the installed capacity, at higher installed capacity lower the specific costs. Figure 7 also shows the specific costs per capita, indicating that for lower population, higher cost per inhabitant is required.

If decision makers want to implement the gasification technology in Icelandic cities, a viable solution for the subgroups 1–5 to reduce the specific costs could be to make connection between neighbour municipalities by making commons investments for bigger gasification facilities, where the T&WW of two or three municipalities could be gasified together.

Regarding revenues, they are obtained by commercialization the generated electricity through the T&WW gasification and the WTB fee for the treatment and disposal of T&WW. Table 5 shows the revenues of the sale of electricity, the WTB fee and total revenue for each subgroup. The revenues have a direct relation with the amount of T&WW production and treated per year, since the higher the input waste, the higher the products. The amount of treated T&WW varies from 304.5 ton/year (subgroup 1) to 10,851.5 ton/year (subgroup 35).

Selling of electricity varies from 12.5 k€ (subgroup 1) to 437.5 k€ (subgroup 35) and the gains because of WTB fees for the T&WW treatment, range from 39.6 k€ (subgroup 1) to 1410.7 k€ (subgroup 35). It is worth mentioning that for all subgroups, the incomes obtained with the WTB fee are equivalent to more than 70% of total revenues.

Fig. 6 Percentage shares of total cost for scenario 1

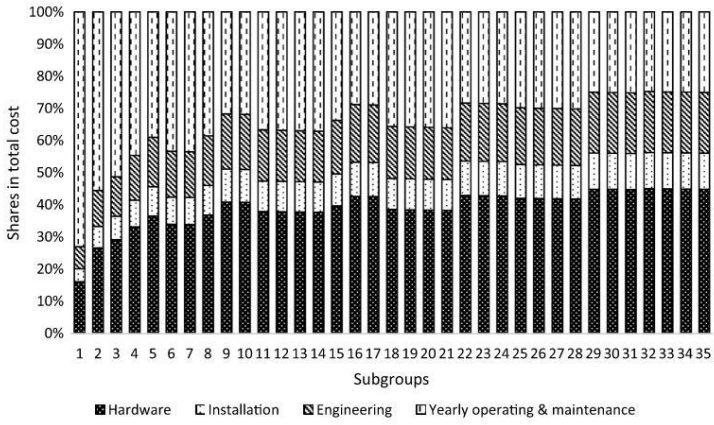

Table 5 The annual revenue based on sale of electricity and waste treated

Subgroups	Income with sale of electricity (k€/year)	Income with WTB (k€/year)	Total income (k€/year)	Subgroups	Income with sale of electricity (k€/year)	Income with WTB (k€/year)	Total income (k€/year)
1	12.50	39.59	52.09	19	237.50	765.47	1002.97
2	25.00	79.91	104.91	20	250.00	805.79	1055.79
3	37.50	120.24	157.74	21	262.50	846.12	1108.62
4	50.00	160.57	210.57	22	275.00	886.44	1161.44
5	62.50	200.89	263.39	23	287.50	926.77	1214.27
6	75.00	241.22	316.22	24	300.00	967.10	1267.10
7	87.50	281.55	369.05	25	312.50	1007.42	1319.92
8	100.00	321.87	421.87	26	325.00	1047.75	1372.75
9	112.50	362.20	474.70	27	337.50	1088.08	1425.58
10	125.00	402.53	527.53	28	350.00	1128.40	1478.40
11	137.50	442.85	580.35	29	362.50	1168.73	1531.23
12	150.00	483.18	633.18	30	375.00	1209.06	1584.06
13	162.50	523.51	686.01	31	387.50	1249.38	1636.88
14	175.00	563.83	738.83	32	400.00	1289.71	1689.71
15	187.50	604.16	791.66	33	412.50	1330.04	1742.54
16	200.00	644.49	844.49	34	425.00	1370.36	1795.36
17	212.50	684.81	897.31	35	437.50	1410.69	1848.19
18	225.00	725.14	950.14				

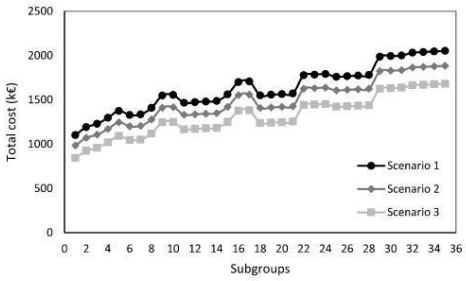

Fig. 8 Total costs for different scenarios

Economic Assessment of Three Scenarios

To have a comparison between different scenarios, the total costs required for power generation based on T&WW gasification, during the period of analysis, for each subgroup are shown together in Fig. 8. Higher interest rates tend to reduce total cost during 15 years of operation. The total costs are as follows, with the interest rate of 8% for Scenario 1 range of 1100 k€ (subgroup 1) to 2050 k€ (subgroup 35), the costs with interest rate of 10% for Scenario 2 range of 983 k€ (subgroup 1) to 1882 k€ (subgroup 35), and total costs with interest rate of 13% for Scenario 3 range of 842 k€ (subgroup 1) to 1680 k€ (subgroup 35). In fact, for the higher interest rate, the smaller present investment is required to achieve the revenue required for the project to succeed. However, the costs alone do not reflect economic-effectiveness of the project. The costs, revenues and their effects together on NPV need to be investigated to demonstrate which project is the most beneficial from the economic perspectives.

The economic assessments, based on the indexes of NPV and DPP for scenarios 1, 2 and 3, are shown in Figs. 9, 10 and 11, respectively. Different from the discount rate, NPVs for three scenarios are positive in 94% of the subgroups (3–35) and negative in the remaining 6% (1 and 2). In other words, implementation of T&WW gasification integrated with power generation unit in Iceland could be economic beneficial projects for places with more than 150 inhabitants or for installed capacities higher than 45 kW. It is worth noting that, in scenario 1 with the interest rate of 8%, NPV is averagely 11% and 25% greater than scenarios 2 and 3, respectively.

In addition, changing the interest rate does not have significant impact on DPP for all studied scenarios; it is lower than 2 years in 88% of the subgroups (5–35) and attractively it is lower than 6 months from subgroup 13 reducing to 4 months for subgroup 35. These all show that employing small-scale T&WW gasification could be an economic alternative in Icelandic municipalities.

The subgroups that do not show economic feasibility for these scenarios could have the strategy of merging in municipalities to reduce the costs and increasing the yields, then

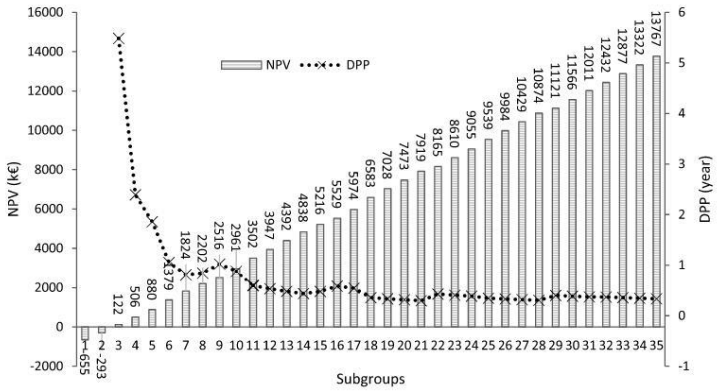

Fig. 9 Economic analysis for scenario 1

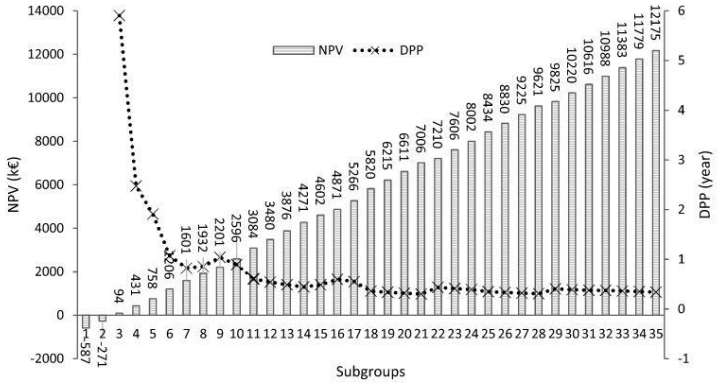

Fig. 10 Economic analysis for scenario 2

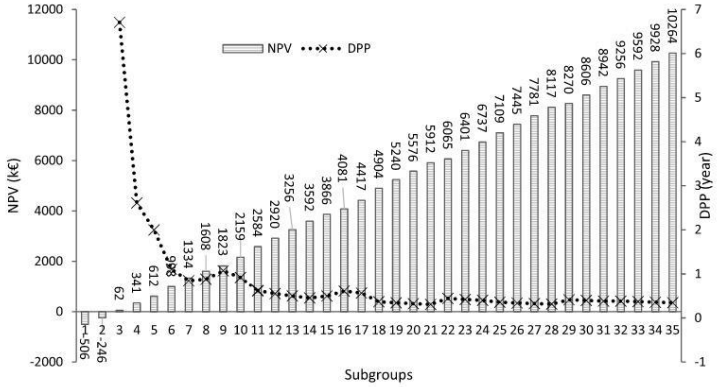

Fig. 11 Economic analysis for scenario 3

looking after the possibility of a higher amount of waste and making viable to install a treatment facility. Another way is to establish a minimum value for the fee of waste collection and disposing. Hence, it was carried out a sensitivity analysis, to find the minimum WTB, to have viable installation of a hypothetical T&WW gasification plant, independent of its size (Table 6). The minimum WTB varies from about 380 € per ton of waste (subgroup 1) for all scenarios to zero from subgroup 14 in scenario 1, subgroup 15 in scenario 2 and subgroup 17 in scenario 3. In other words, in places with more than 700 inhabitants or with the higher installed capacity of 200 kW, projects could be run economically without receiving any fee for collection and disposal of waste.

Environmental Assessment

The environmental impact assessment of timber and wood waste gasification integrated with power production unit is analysed with three categories of global warming, acidification and eutrophication potentials. tonCOThe GWP of T&WW gasification for 35 studied subgroups and average GWP contributions through the gasifying are shown in Fig. 12. It is clear that as the household numbers/population grow, the electricity consumptions increase, therefore greenhouse gas emissions (GHG) are increased. The GHG emitted through T&WW gasification is around 13 tonCO_{2eq} (Subgroup 1) to 469 $_{2eq}$ (Subgroup 35), yearly.

The largest contribution in GWP is made by transport through the consumption of the diesel fuel following with gasifier in conversion step and cutting, handling and drying in the preparation process. Of the process in the chain, conversion 2 containing combustion chamber, gas and steam turbines occupies the smallest share in GWP contributions because when biomass is burnt, carbon dioxide releases back to the atmosphere but this biogenic CO_2 is not counted as a contributor to global warming.

The acidification and eutrophication impacts for T&WW gasification for all studied cases are shown in Fig. 13. Regarding AP index, production of electricity from timber and wood waste gasification creates 173.6 tonSO_{2eq} (Subgroup 1) to 6187.2 tonSO_{2eq} (Subgroup 35) per year. Moreover, electricity generation through the T&WW gasification releases 331.9 tonNO_{3eq} (Subgroup 1) to 11,827.7 tonNO_{3eq} (Subgroup 35), annually. The most important contribution for AP and EP impacts is made by the emissions of particulate matters through the transport sector, following by pre-process and conversions steps (Fig. 13).

Conclusions

In this paper, power supply chain by using timber and wood waste gasification has been analysed and assessed from the technical, economic and environmental perspectives. The technical assessment focused mainly on input waste, installed power, and electrical power generation. The economic assessment conducted relied on the economic indicators of total cost, specific costs, revenues, NPV and DPP, bringing together three different economic scenarios, with interest rates of 8% for Scenario 1, 10% for Scenario 2 and 13% for Scenario 3. Additionally, a sensitivity analysis was carried out, to investigate the effects

Table 6 Minimum WTB for treatment of T&WW to get a NPV more than zero

	Minimum WTB (k€/ton)		
Subgroup	Scenario 1	Scenario 2	Scenario 3
1	0.381	0.384	0.387
2	0.186	0.188	0.192
3	0.115	0.117	0.120
4	0.082	0.084	0.087
5	0.063	0.065	0.069
6	0.043	0.045	0.047
7	0.032	0.033	0.035
8	0.026	0.027	0.029
9	0.025	0.026	0.029
10	0.018	0.020	0.022
11	0.010	0.011	0.013
12	0.006	0.007	0.008
13	0.003	0.003	0.005
14	From 14 to 35 is zero	0.001	0.002
15		From 15 to 35 is zero	0.001
16			0.003
17			From 17 to 35 is zero

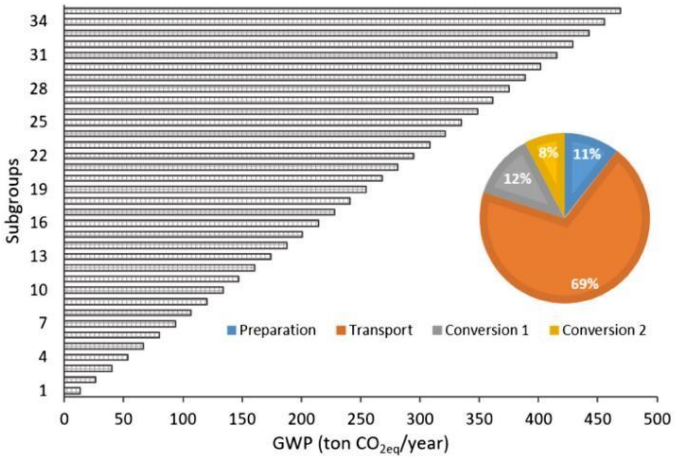

Fig. 12 GWP of T&WW gasification for electricity production and GWP contributions

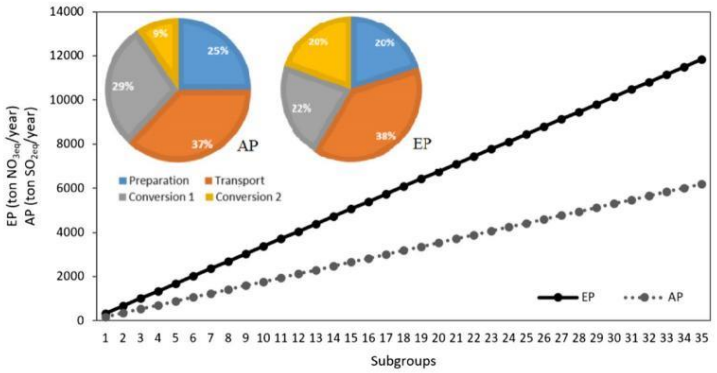

Fig. 13 AP and EP of T&WW gasification for electricity production, AP and EP contributions

of the fee paid by the Icelandic municipalities for collection and disposal of wastes (WTB). The environmental analysis was also directed based on the environmental impacts of global warming, acidification and eutrophication potentials.

We clustered Icelandic municipalities with population lower than 2000 to 35 subgroups based on various number of households/inhabitants. In each subgroup, the study was conducted over hypothetical cases, according to the number of households as each household includes five persons. The costs of equipment, installation, engineering, operation and maintenance and the interest rate of the investment were considered. Regarding revenues, they come from of the electricity sale and the fee paid by the Icelandic municipalities for collection and disposal of waste.

The results show that changing the interest rate does not have significant impact on NPV and DPP for all studied scenarios. The NPV is positive for the municipalities with more than 30 households/150 inhabitants or for a hypothetic gasification plant with the capability to generate greater than 45 kW (for subgroups 3–35). The NPV in scenario 1 (8% for interest rate) is averagely 11 and 25% higher than scenarios 2 and 3, respectively. Moreover, for all studied scenarios, DPP is lower than 2 years in 88% of the subgroups as well as lower than 6 months for 60% of them.

The economic assessment could be also feasible for subgroups (1 and 2), because the WTB fee paid by the Icelandic municipalities for collection and disposal of waste and the quantity of waste can be adjusted. They also can merge together for making viable to install a treatment facility.

Regarding environmental assessment, electricity generation based on T&WW gasification would lead to a GWP of 13 tonCO_{2eq} (Subgroup 1) to 469 tonCO_{2eq} (Subgroup 35), AP of 173.6 tonSO_{2eq} (Subgroup 1) to 6187.2 tonSO_{2eq} (Subgroup 35), and EP potential of 331.9 tonNO_{3eq} (Subgroup 1) to 11,827.7 tonNO_{3eq} (Subgroup 35), yearly. Of the process in the chain, the largest contribution for all impacts is made by transport through the diesel fuel consumption following with gasifier in conversion step and cutting, handling and drying in preparation process.

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Compliance with Ethical Standards

Conflict of interest All authors declare that they have no conflict of interest.

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Paper IX

Techno-Economic Analysis of Power Production by Using Waste Biomass Gasification.
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Techno-Economic Analysis of Power Production by Using Waste Biomass Gasification

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Abstract

Energy recovery from waste biomass can have significant impacts on the most pressing development challenges of rural poverty and environmental damages. In this paper, a techno-economic analysis is carried out for electricity generation by using timber and wood waste (T & WW) gasification in Iceland. Different expenses were considered, like capital, installation, engineering, operation and maintenance costs and the interest rate of the investment. Regarding to revenues, they come from of the electricity sale and the fee paid by the Icelandic municipalities for waste collection and disposal. The economic feasibility was conducted based on the economic indicators of net present value (NPV) and discounted payback period (DPP), bringing together three different subgroups based on gasifier capacities, subgroup a: 50 kW, subgroup b: 100 kW and subgroup c: 200 kW. The results show that total cost increases as the implemented power is increased. This indicator varies from 1228.6 k€ for subgroups a to 1334.7 k€ for subgroups b and 1479.5 k€ for subgroups c. It is worth mentioning that NPV is positive for three subgroups and it grows as gasifier scale is extended. NPV is about 122 k€ (111,020 $), 1824 k€ (1,659,840 $) and 4392 k€ (3,996,720 $) for subgroups a, b and c, respectively. Moreover, DPP has an inversely proportional to the installed capacity. It is around 5.5 years (subgroups a), 9.5 months (subgroups b) and 6 months (subgroups c). The obtained results confirm that using small scale waste biomass gasification integrated with power generation could be techno-economically feasible for remote area in Iceland.

Keywords

Waste Biomass Gasification, Techno-Economic Analysis, Power Production, Waste to Energy

1. Introduction

The rapid development of global economy, increasing population and living standards has been posing great pressure on energy resources and the environment. There is an urgency to use local renewable energies to promote local development and also reduce carbon emission. Waste biomass is an abundant and renewable energy that creates low net CO_2 emission. It is also the only suitable and primary energy resource that can provide transportation fuels [1] [2] [3]. Biomass gasification is an attractive option that is getting huge attention for conversion of different feedstocks to energy. In the gasification, a partial oxidation at elevated temperature (600˚C - 1700˚C) is happened that converts organic components to a Synthesis Gas (syngas), consisting mainly of CO, H_2, CH_4, tars, inorganic impurities and particulates [4] [5].

Beneficially, waste biomass gasification can be applied for small/medium scales that lead to dramatic reduction of some pollutants emission as furans, dioxins, and NOx and the possibility of the utilization of the syngas in high efficiency thermal devices like internal combustion engine and gas turbines [6]. Hence, waste biomass gasification can be installed as a reliable energy supply technology for places which are far from the central energy networks and require district heat and power systems [7] [8] [9].

In this paper, we will explore the potential of timber and wood waste (T & WW) gasification for energy production in small communities in Iceland, (T & WW is the most existing biomass feedstock in this country). In this way, a techno-economic analysis of T & WW gasification facilities integrated with electricity generation unit will be directed for three subgroups with different gasifier installed power, 1): 50 kW, 2): 100 kW and 3): 200 kW to propose a sustainable waste to power system adapted with conditions in Iceland.

2. Material and Methods

2.1. Process Description

Figure 1 shows the studied system in this paper. T & WW is the significant resource entering to the system, liquid fuel and electricity are also the accessory inputs. The proximate and elemental analyses of T & WW are shown in Table 1.

T & WW is transferred from the waste fields to pre-processing part that is next to gasification and electricity generation unit. Diesel fuel is used in trucks

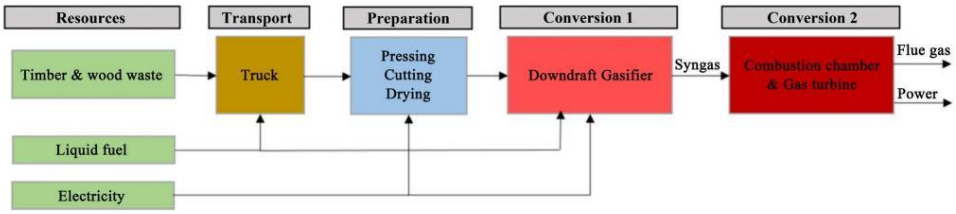

Figure 1. System boundaries, technologies, energy and material streams.

Table 1. Ultimate and proximate analysis of T & WW [10].

Parameters	Value (%)
Proximate analysis (wt%)	
Moisture	5.01
Volatile matter (VM)	93.06
Fixed carbon (FC)	6.38
Ash	0.56
Ultimate analysis (wt%-dry basis)	
C	56.8
H	7.28
N	0.18
Cl	0.82
S	0.07
O	34.29

for transportation and electricity is applied for driving force and heat generation over the process. The electricity production in Iceland is derived from geothermal and hydropower that makes Iceland's main source of clean energy. The gasification process consists of drying, pyrolysis, combustion and gasification [11]. In this work the down draft reactors are considered that operate at atmospheric pressure, to gasify T & WW and air is used as the gasification agent, resulting in CO_2 and H_2O, which subsequently undergo reduction upon contact with the char produced from pyrolysis. Reduction yields combustible gases as H_2, CO, and CH_4 through a series of reactions [5] [12]. Then the produced syngas enters a combustion chamber followed by a gas turbine. The combination of these two modules represents the behavior of a combustion engine where the reaction with air occurs [13] [14]. The inputs values and key assumptions used in this work are based on our waste biomass gasification simulation model developed by ASPEN Plus [8] and the main values of the downdraft gasifiers characteristics, operational parameters and the flue gas composition are relied on our previous work [15].

2.2. Techno-Economic Assessment

In the economic assessment, all prices are expressed in K€ (kilo-euro) and the interest rate is 8%. A computer program has been developed to investigate economically for three subgroups of 50 kW, 100 kW and 200 kW of gasifier installed power. The model is able to evaluate the cash flow analysis, total cost, Net Present Value (NPV) and Discounted Payback Period (DPP). A project is an economically attractive while it has the lowest DPP and the NPV higher than zero. NPV is calculated based on Equation (1) [16]:

$$NPV = \sum_{n=1}^{t} \frac{CF_n}{(1+r)^n} - C_c \quad (1)$$

where CF_n is the annual cash flow, being the difference between Revenues (R)

and Expenditures (E), Operation and Maintenance Costs ($C_{O\&M}$), r is the discount rate, C_c is the total capital costs of investment and t is the lifetime of the investment (15 years). DPP is calculated according to Equation (2):

$$DPP = \frac{LN\left(\frac{1}{1-\frac{C_c \times r}{CF}}\right)}{LN(1+r)} \quad (2)$$

The periodic cash flow, with all the revenues and expenditures, is calculated by considering the incomes from the generated electricity, and the credits for the Waste Treatment Bill (WTB) [6]. The expenditures also include the C_c and $C_{O\&M}$. C_c is divided into three categories: hardware price (C_g), installation cost (25% of C_g) and engineering costs, the engineering costs includes engineering and design (13% of C_g), purchasing & construction (14% of C_g), fuel handling/preparation (9% of C_g) and electrical/balance of plant (6% of C_g) [17] [18]. C_g is the price of gasifier system overally on the basis of various capacities. In this work, we extracted gasifier prices from various companies [19] [20]. C_g was considered 73.6 k€, 105.5 k€ and 147.5 k€ for 50 kW, 100 kW and 200 kW, respectively.

The whole yearly $C_{O\&M}$ can be determined by the sum of the costs for the maintenance cost (2% of C_c), insurance and tax (2% of C_c), waste disposal (15% of C_c), electricity cost, liquid fuel cost and personnel cost. Electricity costs are calculated based on electricity consumers and liquid fuel costs are estimated for fuel consumers with 7000 hr/year of plant availability [17] [18]. The unitary cost of electrical and fuel energies supplied in Iceland are equal to 0.03 $/kWh and 1.08 $/lit (0.91 €/$ as conversion rate) [3]. Personnel cost includes annual labour, cost. A total of two employees were assumed for plant operation management (1 person/shift and 2 shifts/day), with a yearly cost of 60,000 €/year per person in Iceland.

In relation to revenues, the selling price of electricity to normal households and small businesses in Iceland is about 124.69 $/MWh [21]. Hence, the sale price of the generated electricity based on waste gasification was considered at 109.89 $/MWh (100 €/MWh) in our work. Moreover, The Icelandic municipalities pay a fee (WTB) by weight, to the private companies, for the collection and disposal the MSW in sanitary landfills. The WTB for collection and disposal of the MSW varies from 90 - 170 €/ton through over Iceland. In this work, a mean value of 130 €/ton is used.

3. Results

Figure 2 shows the relation between the installed power and the amount of T & WW that is fed to the system for treatment and power production. Clearly, as the installed power grows, input biomass also increases. The requested waste biomass varies from 132.1 kg/hr for the first subgroup to 309.5 kg/hr for the second one and 575.3 kg/hr for the third subgroup.

The total cost of the generation plant for each subgroup is shown in Figure 3. The total cost increases as the installed power grows, it is about 1228.6 k€ (Subgroup a), 1334.7 k€ (Subgroup b) and 1479.5 k€ (Subgroup c). In addition, Figure 4 depicts the percentage shares of hardware, installation, engineering and annual

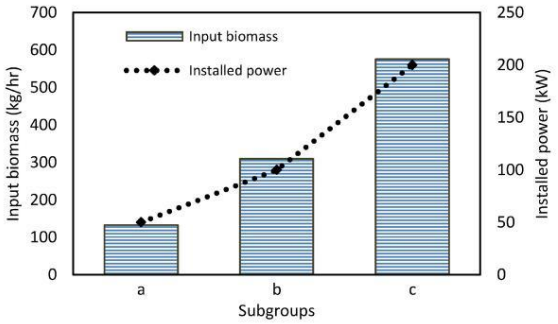

Figure 2. Input T & WW and installed power for subgroups.

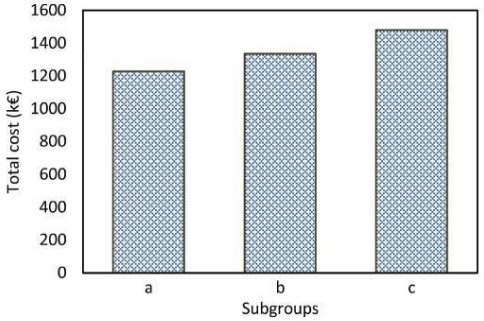

Figure 3. Total costs for different subgroups.

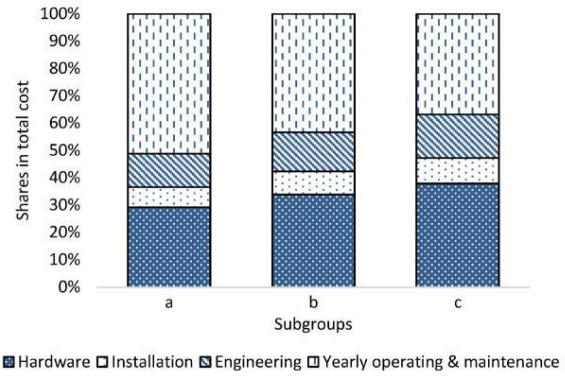

Figure 4. Percentage shares of total cost.

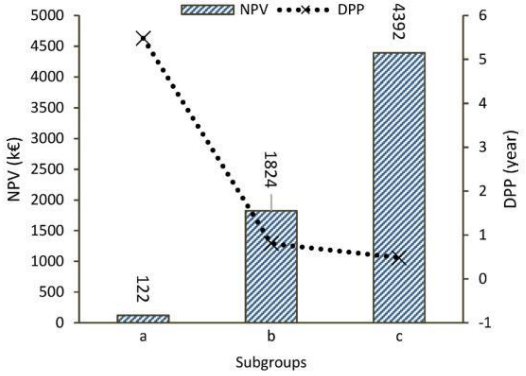

Figure 5. NPV and DPP for different subgroups.

O & M costs in total cost. The yearly O & M costs occupies more than 55% of total cost for the first subgroup, it has also the dominant statue among different kinds of costs for subgroups b (43%). However, the highest share is related to gasification system price for subgroups c.

The economic assessments, based on the indexes of NPV and DPP for three subgroups, are shown in **Figure 5**. It is worth mentioning that NPV is positive for three subgroups and it grows as gasifier scale is extended. NPV is about 122 k€, 1824 k€ and 4392 k€ for subgroups a, b and c, respectively. Moreover, DPP shows the gasification plant in this context is very feasible for Iceland. It has an inversely proportional to the installed capacity. It is around 5.5 years (subgroups a), 9.5 months (subgroups b) and 6 months (subgroups c).

4. Conclusion

In this work, techno-economic of power production plant that utilized syngas from a timber and wood waste gasification process in Iceland was investigated. The technical assessment focused mainly on input waste, and installed power. The economic assessment was conducted relied on the economic indicators of total cost, revenues, NPV and DPP, for three subgroups with different gasifier installed power, 1): 50 kW, 2): 100 kW and 3): 200 kW. The results show that total cost increases as the implemented power is increased. This indicator varies from 1228.6 k€ for subgroups a to 1334.7 k€ for subgroups b and 1479.5 k€ for subgroups c. It should be emphasized that NPV is positive for three subgroups and it grows as gasifier scale is extended. The NPV in subgroup c, is averagely 58% and 97% higher than subgroups b and a, respectively. NPV is about 122 k€, 1824 k€ and 4392 k€ for subgroups a, b and c, respectively. Moreover, DPP has an inversely proportional to the installed capacity. It is around 5.5 years (subgroups a), 9.5 months (subgroups b) and 6 months (subgroups c). Finally, the obtained results confirm that using small scale waste biomass gasification integrated with power generation could be techno-economically feasible for remote area in Iceland.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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Paper X

Performance analysis of power generation by wood and woody biomass gasification in a downdraft gasifier.
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Performance analysis of power generation by wood and woody biomass gasification in a downdraft gasifier

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ABSTRACT

An equilibrium simulation model was developed by applying Aspen Plus to evaluate the performance of 28 wood and woody biomass (W&WB) gasification in a downdraft gasifier integrated with power production unit. The developed simulation model does not focus the gasification process as a closed box, it considers important processes in gasification like drying, pyrolysis, combustion, gasification and integrated with power production plant (combustion chamber plus gas turbine). The results for the 28 W&WB alternatives show that the net power produced from 1-ton feedstock entering to the gasification system is between the interval [0-400 kW/ton] and among them, gasification system derived from Tamarack bark biomass significantly outranks all other systems by producing 363 kW/ton, owing to the favorable results obtained in the performance analysis. Moreover, effect of various operating parameters such as gasification temperature and air to fuel ratio (AFR) on the system performance was carried out. Finally, the developed model is applied as an effective tool to assess the impact of so many biomasses and operating parameters on output power.

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1. INTRODUCTION

The finite nature of fossil fuels, high prices and their negative effects on environment and public health, are encouraging to find renewable energy sources and alternative technologies to produce power [1-3]. Biomass is a renewable energy option that is abundant and can create low net CO_2 emission and it has also the greatest potential to substitute for transportation fuels [4-7]. Woody biomass is also one of the important energy sources and it is currently the most important source of renewable energy, globally. In 2010 worldwide use of woody biomass as energy resource was about 3.8 Gm^3 (30 EJ/year), which consisted of 1.9 Gm3 (16 EJ/year) for household fuel wood and 1.9 Gm^3 (14 EJ/year) for large-scale industrial sector. During this period, global primary energy consumption and global renewable energy consumption were 541 EJ and 71 EJ, yearly. Hence, in 2010 woody biomass formed roughly 9% of world primary energy consumption and 65% of world renewable primary energy consumption [8, 9].

Gasification has attracted attention as one of the most efficient methods for utilizing woody biomass, as CO_2 emission has become an important global issue [10-14]. Biomass gasification means incomplete combustion of biomass resulting in production of combustible gases consisting of carbon monoxide (CO), hydrogen (H_2) and traces of methane (CH_4) [15-20]. This mixture is called syngas. Syngas can be used directly to run internal combustion engines, it can be consumed as substitute for furnace oil for

heat production and can be used as chemical feedstock to produce methanol [21-25]. Therefore, the development of small-scale, woody biomass gasification is a great social need in a resource-poor country or for regions which are far from the central energy networks and require district heat and power systems [11, 26, 27]. The primary aim of this work is to develop a steady state computer model by using Aspen Plus for performance analysis of 28 wood and woody biomass (W&WB) gasification in a downdraft gasifier integrated with power production. The objective is to find the most efficient W&WB for power production. Then as a sensitivity analysis we examine the effect of operating parameters of temperature and air to fuel ratio (ARF) to know where the overall system is optimal to reach the maximum net output power.

2. MATERIAL AND METHODS

A simulation model relied on equilibrium approach is developed for wood and woody biomasses (W&WB) gasification linked with power generation plant by employing Aspen Plus. In order to compute physical properties of the components in the gasification, equation of state of PR-BM, Penge Robinson-Boston-Mathias alpha is applied. In addition, for modeling of enthalpy and density of biomass and ash as non-conventional materials, HCOALGEN and DCOALIGT models are used. It is worth to say that MCINCPSD stream includes 3 streams of MIXED, NCPSD & CIPSD classes, to define the biomass structure and ash streams that are not in Aspen Plus database [12, 28-33]. Figure 1 shows the flow chart of the system simulated in Aspen Plus. The feedstock stream has been described as a nonconventional material and it was defined by determination of the elemental and proximate analysis of feedstock. In order to have a detailed study, 28 W&WB were considered as feedstock for gasifier. Table 1 shows the proximate and elemental analyses of all these feedstocks [34-49]. Temperature through the drying is around 150 °C to reduce moisture of the original biomass to less than 5 wt%. This step is done by utilizing a RSTOIC, stoichiometric reactor in Aspen Plus. RSTOIC module is practical for chemical reactions with known stoichiometry [50-51].

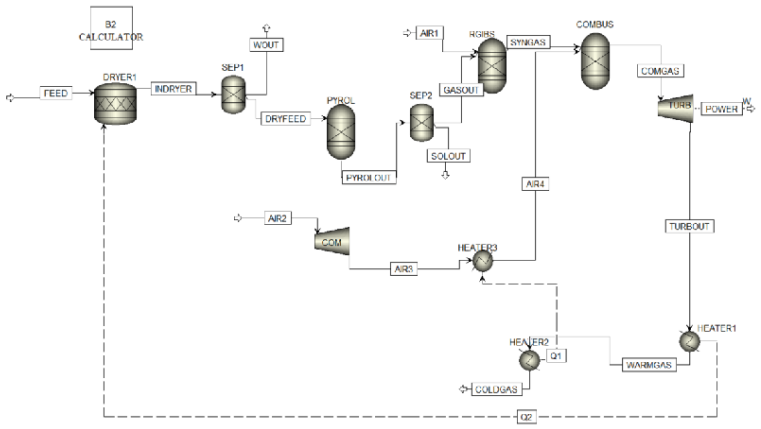

Figure 1. Modules and streams of gasification simulated in Aspen Plus

At the next stage, RYIELD, the yield reactor is simulated for feed pyrolysis. In this part, the studied biomass is transformed to volatile materials (VM) and char. VM includes mainly carbon, hydrogen, oxygen and nitrogen. Char also includes ash and carbon [12, 52-56]. After pyrolysis, RGibbs is applied for simulation of the biomass gasification. This reactor computes the syngas composition by minimizing the Gibbs free energy based on complete chemical equilibrium assumption [57-61]. Input streams to the RGibbs are decomposed biomass and air then combustion and reduction reactions will be occurred inside of the reactor. For combustion level, another RGibbs reactor needs to be simulated with minimum air mixing. This process will be also based on minimization of Gibbs free energy. To generate power, the combustion chamber has to be connected with a gas turbine [62-66]. The thermal content of the flue gas, achived as the combustion heat is recovered to preheat the input air to the combustion chamber as well as to supply the heat required in dryer. The recovered heat can be also utilized for convertion of water to high pressure steam to be

able generates extra power by steam driving a steam turbine [40, 41] (this part was not considered in this study). The solid lines and the dashed lines in the Figure 1 present the mass streams and heat streams, respectively. The system is also assumed to be auto-thermal that means a part of the feedstocks is combusted inside the gasifier to provide the heat required in situ. Heat is also obtained by the hot syngas and the combustion chamber then it is consumed wherever required.

Table 1. Elemental and proximate analysis of 28 wood and woody biomasses [20-35]

		Proximate analysis (wt%)				Elemental analysis (wt%- dry basis)				
		M	VM	FC	A	C	O	H	N	S
1	Alder-fir sawdust	52,6	76,6	19,2	4,2	50,9656	38,5116	5,8438	0,479	0
2	Balsam bark	8,4	77,4	20	2,6	52,596	38,473	6,0388	0,1948	0,0974
3	Beech bark	8,4	73,7	18,5	7,8	47,3908	38,5396	5,532	0,6454	0,0922
4	Birch bark	8,4	78,5	19,4	2,1	55,803	34,9503	6,5593	0,4895	0,0979
5	Christmas trees	37,8	74,2	20,7	5,1	51,7205	36,7263	5,5991	0,4745	0,3796
6	Elm bark	8,4	73,1	18,8	8,1	46,7771	39,0575	5,3302	0,6433	0,0919
7	Eucalyptus bark	12	78	17,2	4,8	46,3624	43,1256	5,4264	0,2856	0
8	Fir mill residue	62,9	82	17,5	0,5	51,143	42,2875	5,97	0,0995	0
9	Forest residue	56,8	79,9	16,9	3,2	51,0136	39,7848	5,2272	0,6776	0,0968
10	Hemlock bark	8,4	72	25,5	2,5	53,625	37,83	5,7525	0,195	0,0975
11	Land clearing wood	49,2	69,7	13,8	16,5	42,3345	35,738	5,01	0,334	0,0835
12	Maple bark	8,4	76,6	19,4	4	49,92	39,648	5,952	0,384	0,096
13	Oak sawdust	11,5	86,3	13,4	0,3	49,9497	43,7683	5,8823	0,0997	0
14	Oak wood	6,5	78,1	21,4	0,5	50,347	42,6855	6,0695	0,2985	0,0995
15	Olive wood	6,6	79,6	17,2	3,2	47,432	43,4632	5,2272	0,6776	0
16	Pine bark	4,7	73,7	24,4	1,9	52,7778	39,1419	5,7879	0,2943	0,0981
17	Pine chips	7,6	72,4	21,6	6	49,632	38,07	5,734	0,47	0,094
18	Pine pruning	47,4	82,2	15,1	2,7	50,4987	40,1849	6,1299	0,4865	0
19	Pine sawdust	15,3	83,1	16,8	0,1	50,949	42,8571	5,994	0,0999	0
20	Poplar	6,8	85,6	12,3	2,1	50,5164	40,8243	5,9719	0,5874	0
21	Poplar bark	8,4	80,3	17,5	2,2	52,4208	38,4354	6,5526	0,2934	0,0978
22	Sawdust	34,9	84,6	14,3	1,1	49,2522	43,2193	5,934	0,4945	0
23	Spruce bark	8,4	73,4	23,4	3,2	51,8848	38,72	6,0016	0,0968	0,0968
24	Spruce wood	6,7	81,2	18,3	0,5	52,0385	40,994	6,0695	0,2985	0,0995
25	Tamarack bark	8,4	69,5	26,3	4,2	54,606	30,656	9,7716	0,6706	0,0958
26	Willow	10,1	82,5	15,9	1,6	49,0032	42,7056	6,0024	0,5904	0,0984
27	Wood	7,8	84,1	15,7	0,2	49,5008	44,0118	6,0878	0,0998	0,0998
28	Wood residue	26,4	78	16,6	5,4	48,6244	39,6374	5,7706	0,473	0,0946

3. RESULTS AND DISCUSSION

The simulation model results for the 28 W&WB alternatives, ranked regarding their contribution to output net power ($W_{net} = W_{gas\ turbine} - W_{compressor}$) for 1 ton feedstock are shown in Figure 2. This ordering is based on the net power that it is between the interval [0-400 kW/ton], values highlighting the lowest and the highest efficient options, respectively. Class 1 includes 5 wood and woody biomass gasification systems based on Land clearing wood, Fir mill residue, Forest residue, Eucalyptus bark and Alder-fir sawdust that produce the lowest amounts of output power (it is in the range of 0-100 kW/ton). Many of the studied W&WB gasification systems are located in class 2 which their output power is in span of 100-200 kW per one tone of feedstock. Class 3 contains 7 wood and woody biomass gasification systems relied on Spruce wood, Pine bark, Spruce bark, Balsam bark, Hemlock bark, Poplar bark and Birch bark which generate relatively higher net power.

Obviously, the gasification system derived from Tamarack bark biomass significantly outranks all other systems from the viewpoint of power production (363 kW/ton), owing to the favorable results obtained in the performance analysis. This is mainly due to Tamarack bark has the highest percentage of carbon and hydrogen, see Figure 3. Percentage shares depicted in Figure 3 are contributions of carbon and hydrogen, oxygen, ash and nitrogen and sulphur in elemental analysis of each feedstock. Carbon and hydrogen are key elements in each biomass. So that the higher C and H_2 content, the more carbon monoxide and hydrogen will be in the syngas and also leads to the improvement of heating value (LHV) of syngas. CO and H_2 are combustible substances which are converted to flue gas (mainly CO_2 and H_2O) through the combustion chamber. Therefore, improving LHV of syngas leads to enter gases at high temperature to the gas turbine. Raising the turbine inlet temperature ameliorates output power from that as well as more net power will be resulted.

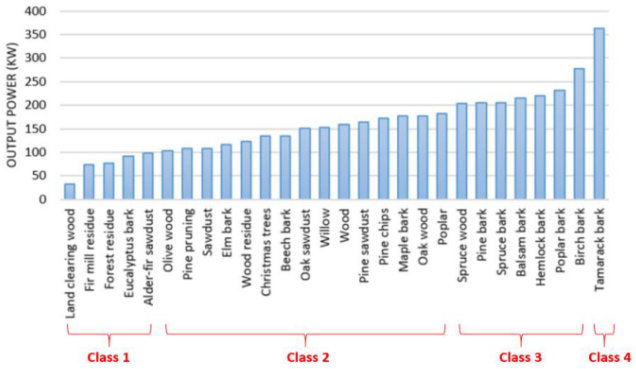

Figure 2. Net output power from 28 W&WB gasification systems based on 1 ton feedstock (gasifier temperature 900 ˚C and air to fuel ratio 2)

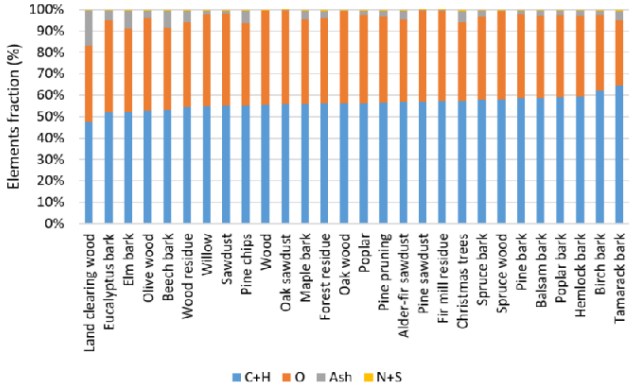

Figure 3. Percentage shares of composing elements for different W&WBs

The impact of temperature of gasifier on power generated from the 28 wood and woody biomass gasification systems, is presented in Figure 4. The sensitivity results in Figure 4 are all at fixed conditions of 1-ton biomass input, air to fuel ratio (AFR) of 2 and temperature of gasifier in the range of 600-1500 ˚C. Obviously for all studied W&WBs, output power from each system is increased by growing temperature. At low temperature (600 ˚C), the present carbon in the feedstock is not completely oxidized, so the syngas product can not be in an acceptable quantity. In fact, at low temperature, CH_4 and unburned carbon will stay in syngas then by growing temperature much more carbon is combusted and transformed to CO relied on partial combustion reaction. CH_4 is also converted into H_2 by reverse methanation reaction. Moreover, water gas reaction (WG) moves toward CO and H_2 production at high temperature. So, increasing the temperature of gasifier is so proper for H_2 and CO production which causes to the improvement of lower heating value (LHV) of product gas. Then, modified LHV of syngas makes higher quality gases entering to the combustion chamber as well as high temperature gasses entering to the gas turbine. Consequently, growing TIT, turbine inlet temperature increases power output from the system. However, at a specific temperature, yield of H_2 and CO are satisfied, both reach to an approximately fixed rates that is called the optimum temperature for the gasifier. Output power also increases in a gradual way near the optimum temperature. The optimum temperature of the down draft gasifier for W&WB is in the range of 900-1000 ˚C.

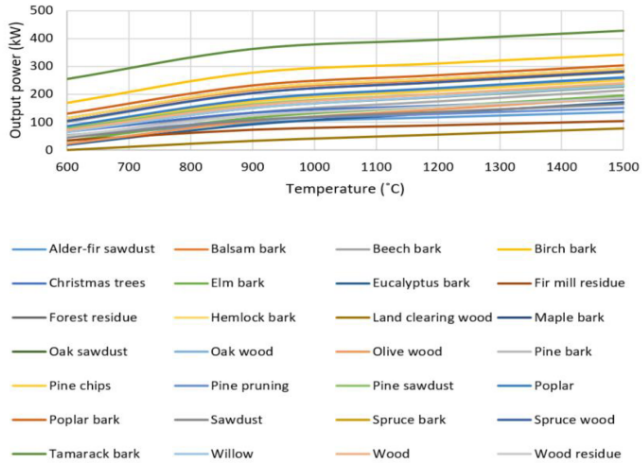

Figure 4. Impact of temperature of gasifier on power for 28 W&WBs

Changes in the air values used in the system have a critical impact on the quality and composition of the product gas and following the generated power. The amont of air arriving the gasifier can be represented in the form of air to fuel ratio (AFR), which is the amount of air needed to burn a unit of dry biomass. The effect of AFR on power produced for the gasification systems derived from 28 wood and woody biomasses, is shown in Figure 5. In this assessment, the operating conditions are fixed on gasifier tempretare of 900 ˚C and 1 ton from each feedstock. The optimum AFR for W&WB gasification is between 1,8-2. At low AFR, biomass reactions will approach to the pyrolysis, charcoal remains with corresponding energy losses. However, at much amount of AFR the additional oxygen is reacted that caused the reduce in syngas production. So, it is critical to find the proper range of AFR for W&WB gasification.

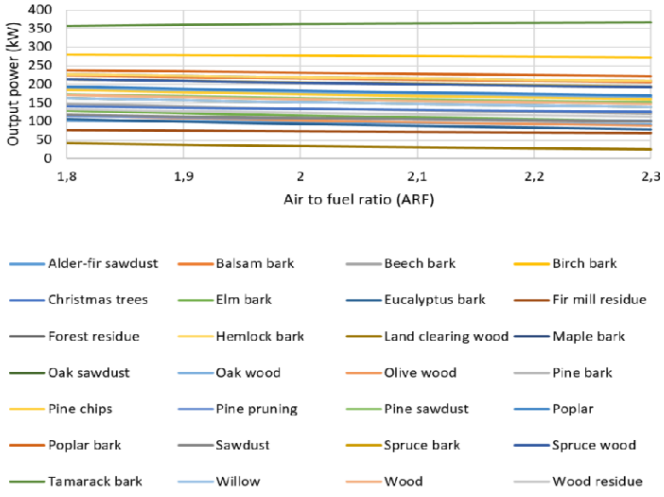

Figure 5. Effect of AFR on output power for 28 W&WBs

4. CONCLUSION

An integrated gasification simulation model is developed containing a series of modules that models processes individually through the gasification of biomass. These processes are drying, pyrolysis, combustion and gasification linked with power generation plant (combustion chamber plus gas turbine). The established model is relied on thermodynamic equilibrium approaches and it is employed for 28 wood and woody biomasses. The studied model is practical for prediction of some outputs such as net power in a variety operating conditions like air flow rate and temperature and for different kinds of biomass materials with a specified ultimate and proximate analysis. The extablished simulation model can be a helpful tool for principally evaluation, assessment, and operation of down draft biomass gasifiers. Furthermore, the model can be employed as an assessment of various alternatives at an early stage to allow the decision-makers to carry out efficient oriented decisions.

The simulation model results for the 28 W&WB alternatives show that the net power produced from 1-ton feedstock entering to the gasification system is between the interval [0-400 kW/ton] and among them, gasification system derived from Tamarack bark biomass significantly outranks all other systems by producing 363 kW/ton, owing to the favorable results obtained in the performance analysis. At the end, a sensitivity analysis was directed to evaluate the influence of temperature of gasifier, and AFR on output power production from each system. Extention of temperature modifies the gasifier performance, it grows the production of both CO and H_2 that causes to higher power on output. While, growing AFR reduces CO and H_2 production which makes in degrading of system performance.

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